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## TRANSACTIONS A: BASICS

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Materials and Energy Research Center

In the Name of God

## INTERNATIONAL JOURNAL OF ENGINEERING **Transactions A: Basics**

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# A New Comprehensive Model for Integrating Environmental, Economic, and Social Performance of Deep and Large-scale Open-Pit Copper Mines

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#### PAPER INFO

## ABSTRACT

Paper history: Received 05 August 2023 Received in revised form 12 September 2023 Accepted 13 September 2023

Keywords: Sustainability Assessment Deep and Large-scale Open-Pit Copper Mine Environmental Impact Economic Impact Social Impact Scenarios Deep and large-scale (D&LS) open-pit mines pose various environmental, social, and economic impacts on the mining projects' stakeholders and local, regional, national, and international communities. Identifying these impacts and having a comprehensive model to assess these impacts altogether is critical to achieving sustainable development (SD) goals. This study develops a robust sustainability assessment model for D&LS open-pit mining projects. The model comprehensively considers 99 impact factors across environmental, social, and economic dimensions. The sustainability score is calculated using the Z-FDAHP technique to reduce the bias and uncertainty of experts' judgments. Then, the scenario-based technique is used to apply the stakeholders' perspective to the model. The model is applied to Sungun Copper Mine (SCM) in northwest Iran for verification. Results show SCM's sustainability performance is highly sensitive to index weightings. The highest score was achieved with sole social prioritization (scenario 8 with a sustainability score of 6.364 out of 10), highlighting the critical role of community impacts. Environmental or economic focus alone (scenarios 2 and 5) was not very sustainable, with scores of 3.326 and 5.298 respectively. Scores of 5.543, 5.330, and 5.117 for sustainability can be achieved by optimizing all three SD aspects with a long-term, stakeholder-centered approach (scenarios 9, 4, and 6). The proposed sustainability assessment model exhibits robustness through its comprehensive set of 99 environmental, social, and economic indicators; its ability to customize indicator weights under different stakeholder-perspective scenarios; and validation of the quantitative scoring approach through an empirical case study, while continuous improvement would further reinforce its robustness over time.

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#### **1. INTRODUCTION**

Copper mining provides a resource that is important for many industrial uses. Reasons for rising copper demand include a growing world population, greater economic activity, and increased manufacturing of coppercontaining products like power cables, electronics, plumbing, and building materials. Along with the depletion of high-quality, easily accessible copper sources, large-scale mining of lower-grade and deeper copper deposits has become necessary due to this increased demand. However, copper mining, like many minerals other metals and mining, impacts environmental, economic, and social aspects requiring management for sustainable development. Deep and Large-Scale (D&LS) open-pit mines present unique sustainability challenges due to their large scale, high resource throughput, emissions, water usage, land use impacts, and potential effects on communities and ecosystems. These complex projects require thorough, sophisticated analyses to balance mining needs with environmental and social responsibility. However, with careful planning and stakeholder involvement, such operations can help meet increasing copper demand in an environmentally and socially responsible manner while minimizing negative impacts. Numerous scholars have researched the environmental, economic, and social impacts of mining activities.

Vizayakumar and Mohapatra (1) addressed the environmental impacts of coal mining activity. Coal is the primary source of energy in India, but environmental pollution in agricultural areas is very severe. Rybicka (2) examined the environmental impacts of mines in Poland and noted an increasing concentration of pollutants, especially heavy metals, in natural soils and water systems from industrial sources poses a serious threat. Work on defining key parts of Environmental Impact Assessments (EIAs) started with Sadler's 1996 report [3]. He described effectiveness as how well an assessment achieves its intended objectives. Three main types of effectiveness were identified: procedural, material, and financial. Procedural focuses on process structure and policy continuity. The material examines the impact on decision-making and reducing negative environmental impacts. Financial concerns costs and time of EIA (3). Jarvis and Younger (4) studied the EIA of mine water, with pollution from mines being a major water problem in the UK (United Kingdom) and internationally. Kuma et al. (5) researched EIAs in Ghana, proposing an approach for pre-mining groundwater economic and technical impact identification, though neglecting other environmental impacts. Folchi (6) proposed a widely used model to investigate the environmental impacts of open-pit mines, considering only 8 impact factors. The Folchi model has been used by many scholars ever since, but it has a narrow scope and does not account for all impacts (7-9). In 2006, Kitula (10) examined the socioeconomic impacts of mining activities in the Geita district in Ghana. The findings showed that approximately 66% of mining community households' income was derived from the mining industry. Additionally, it was found that less than 5% of Ghana's Gross Domestic Product (GDP) originated from mineral extraction. The small amount added to GDP compared to mining's large local importance means Ghana's mining industry needs more investment. Pandey et al. (11) studied the environmental impacts of the Malanjkhand copper mine in India. They investigated various factors such as acid mine drainage (AMD), impacts on flora and fauna, general environmental pollution, water quality, and impacts on aquatic organisms. Rashed (12) assessed and monitored pollution from the tailings of the Allaqi Wadi Aswan gold mine in southeast Egypt. Aryafar et al. (13) employed a modified Folchi method to assess the environmental implications of the East-Alborz coalwashing plant in northeastern Iran. The researchers used an adapted Folchi approach to analyze the environmental impacts of a coal facility in Iran. Similarly, Northey et al. (14) assessed impacts of copper mining through report data. By using corporate sustainability sustainability reports, they could evaluate the environmental consequences of copper mining operations. Minaei Mobtaker and Osanloo (15) conducted a study examining the potential positive outcomes of mining operations. The research showed mining can provide various economic, social, and environmental benefits based on the evaluation of impacts. Northey et al. (16) evaluated the environmental impacts of copper mining using data from sustainable development reports. They focused on factors like greenhouse gas emissions, fossil fuel consumption, and water consumption. Taušová et al. [17] investigated the socioeconomic impacts of mining over time in Slovakia. Research has found around 4,000 employees work in the Prievidza region directly involved in mining. Additionally, approximately 6,000 more jobs are indirectly supported by or connected to mining activities in the area (17). Amirshenava and Osanloo (18) developed a framework to assess the impact of mining activities on sustainable development indicators. Their model included 14 criteria: 8 environmental criteria. 3 social criteria, and 3 economic criteria. Yankson and Gough (19) studied the influence of gold mining on livelihoods and transformations in the mining scale. The research found that between 2001 and 2011, gold mining contributions to household income increased up to fivefold in certain localities. This suggests mining, particularly artisanal and small-scale gold extraction, played a dramatically heightened economic role for communities over that decade-long period according to the income data analyzed. Von der Goltz and Barnwal (20) conducted an extensive analysis of 800 mines across 44 developing nations, finding mining operations provide considerable long-term economic gains but these are also spatially constrained. They discovered that asset levels were higher for those within 20 km of mines, showing mining wealth mainly stays within close local communities. But for people living farther than 20 km, there was no correlation between mining activity and increased household assets or prosperity. So, while mining boosts local economies, these economic impacts do not spread much past the tight sphere of direct influence around 20 km from mine sites, with the gains mostly confined to nearby local communities close to the mining operations. Argimbaev et al. (21) examined ironbearing tailings from waste dumps at ore processing facilities in the Kursk Magnetic Anomaly region of Russia. Microscope examination from 90-600x magnification revealed varied particle sizes and shapes indicating potential construction uses for tailings after further processing. Tabasi and Kakha (22) evaluate the environmental impacts of granite quarrying activities near Boog, Iran. By quantifying the impacts of factors on designated environmental components with a systematic fuzzy approach, this research assisted in environmental impact assessments for mining projects. Atienza et al. (23) examined the impacts of mining on urban growth in Chile. Through standard econometric analysis, they discovered that real estate investment expansion primarily correlated with mining activity, copper exports, national monetary fluidity, and regional wages. Consequently, mining income in urban areas appears predominantly influenced by household earnings from mining and the subsequent redistribution of this income into property and asset investments. Hosseinpour et al. (24) proposed a framework of 29 positive and negative impacts; but it is not specific to D&LS mines. Cacciuttolo and Cano (25) analyzed the environmental impacts of gold and copper extraction in Chile and Peru, which considered metallurgical processing. Kumar et al. (26) analyzed the geotechnical properties and remediation of contaminated soil from gold mines in Karnataka, India. The research sought to characterize the contaminated mine soil geotechnically and identify a soil-washing method to prevent surrounding environmental pollution. Sanjuan-Delmás et al. (27) evaluated the life cycle environmental impacts of European copper production using SimaPro and GaBi software. Gümüşsoy et al. (28) investigated the economic potential and environmental consequences of extracting metals from copper flotation slag. Song et al. (29) assessed the environmental conditions in mineral-rich areas of China using remote sensing techniques. The impacts of noise and noise control strategies at the large-scale Zijin copper mine in Serbia was evaluated by Pantelic et al. (30). Dust levels in a Chinese coal mine was estimated by Luan et al. (31)

applying machine learning models. Jafarzadeh et al. (32) used numerical modelling to analyze different cover system designs for mine tailing dams in arid regions. The research found that a capillary barrier cover system was most effective at maintaining around 80% saturation in the storage layer, immediately cutting off oxygen diffusion compared to other designs. By optimizing the cover system and controlling oxygen entry parameters, mine waste sites can better reduce AMD. Alsaleh et al. (33) analyzed the effect of geothermal energy output on carbon dioxide emissions across European nations from 1990 to 2021. Heydari et al. (34) proposed a 37-factor social impact assessment model for mining. However, it focuses only on social impacts, not environmental and economic impacts. Heydari and Osanloo (35) proposed a 44-factor environmental impact assessment model for D&LS open-pit mines. In another study, they developed a 28-factor economic impact assessment model (36). The existing studies on the environmental impacts of mining have limitations. None of the research looks at the effects of D&LS open-pit mines comprehensively. The models also do not address all three indexes of sustainable development - environmental, economic, and social - in their assessment. A sustainability model is needed that considers all three dimensions to identify sustainability issues. This type of mine requires a customized sustainability assessment model. The current studies do not fully examine the impacts of D&LS open-pit mines or provide a solution for assessing sustainability in this context by looking at all SD indexes together.

This study aims to (1) combine three separate models for environmental, economic, and social assessment to make a single inclusive sustainability model under different scenarios, (2) calculate a sustainability score for D&LS copper mines from different stakeholders' point of view, and (3) give mine managers and stakeholders a unified tool to inform decisions for more sustainable mining. The model will be verified using the Sungun Copper Mine in Iran.

#### 2. METHODOLOGY

Previous studies proposed individual models for assessing the social, environmental, and economic aspects of copper mine sustainability (34-36). This study combines those three models into one comprehensive sustainability model for D&LS open-pit copper mines. It includes all three sustainable development areas. This helps work towards the Sustainable Development Goals (SDGs). The proposed model involves defining the model scope, collecting data, and getting final results from the three component models, which were developed by the authors. Then it calculates importance weights, scores, and the overall sustainability score. This provides a unified assessment approach. to calculate the sustainability score for each sustainable development (SD) index. Scenarios are then defined to capture various stakeholders' points of view. Finally, the sustainability score for D&LS copper open-pit mines can be determined (see Figure 1).

**2. 1. The Scope** When modeling the sustainability score of a D&LS open-pit copper mine, the following items should be considered as part of the model scope:

- 1. Environmental sustainability: This aspect of the model scope should consider the impact of mining activities on the environment, including air and water quality, land use, and biodiversity.
- 2. Economic sustainability: This aspect should consider the mine's ability to generate economic benefits, such as employment opportunities and



Figure 1. Schematic overview of the proposed model

contributions to local and national economies. The model should also evaluate the costs associated with D&LS open-pit mining, such as waste disposal and remediation.

3. Social sustainability: This aspect of the model scope should consider the mine's impact on the health, safety, and well-being of workers and local communities, as well as its contribution to the development of local infrastructure and social programs. The model should evaluate the mine's performance in terms of labor standards, community engagement, and social responsibility.

By considering these items in the model scope, a comprehensive assessment of the sustainability performance of a D&LS open-pit copper mine can be obtained.

**2. 2. Factors Identification** Identifying factors for a sustainability model of a D&LS open-pit copper mine requires a multidisciplinary approach and the collection of data from various sources. The following are some steps that can be taken to identify the factors for the model:

- 1. Identify the requirements: Based on the items considered in the model scope, identify the requirements for each of the models that need to be considered. The requirements include possible environmental, economic, and social factors.
- 2. Create a list: Create a list by conducting site visits, surveys, and interviews with stakeholders such as mine workers, local communities, and various sources such as company reports, academic papers, government reports, and industry databases.
- 3. Ensure completeness of the list: It is important to ensure the list collected is complete by using reliable sources and validated methods.

No.	Affecting factor	Definition	
1	Overburden	Volume of overburden rock removed to access orebody at depths near 1000m	
2	Waste rock	Volume of waste rock from low-grade orebodies at depths near 1000m	
3	Tailing	Volume of tailings from processing low-grade orebodies mined at depths near 1000m	
4	Waste Management	Reusing mine tailings and managing waste materials	
5	Acid Mine Drainage	Acid mine drainage potential from pyrite in orebody	
6	Ecosystem	Impacts on local biodiversity from habitat loss or fragmentation affecting species	
7	Deforestation	Removing forest canopy to access orebody underneath	
8	Life Below Water	Impacts on aquatic life from polluting nearby water	
9	Ecotoxicity	Toxic impacts and contaminants harming terrestrial and aquatic organisms	
10	Ecosystems amend due to reclamation	Improving ecosystem health through habitat, water, and biodiversity restoration	

**TABLE 1.** Environmental Factors for a Comprehensive Model

11	Topsoil quality	Topsoil removal eliminates organic matter, nutrients, and microbes. Heavy equipment compacts soil reducing porosity and aeration. Waste rock piles degrade soils.
12	Deep soil quality	Soil properties at depth differ from topsoil due to compaction, depletion, and changes from mining.
13	Terrestrial ecotoxicity	Potential soil contamination varies by project scale and waste volumes.
14	Eutrophication	Mining could affect nutrient-rich surface water through mineral and nutrient inputs.
15	Freshwater ecotoxicity	Freshwater ecotoxicity metrics like heavy metals, pH, and sensitive organisms.
16	Surface water quality	Mining introduces pollutants into waterways affecting surface water quality.
17	Underground water quality	Groundwater contamination potential from leaching chemicals and metals from waste/tailings with long-term impacts.
18	Water Table change	Upward water pressure in open pits presents slope stability and safety issues and impedes mining due to poor drainage.
19	Water consumption	Water demand/consumption depends on project technical aspects and site conditions.
20	Water management	Appropriate water management depends on project/site characteristics.
21	Photochemical ozone formation	Ground-level ozone degrades local air quality and risks respiratory health in communities near mining due to emissions from equipment and machinery.
22	Ozone depletion	Stratospheric ozone depletion from mining operations may occur through emissions of chlorofluorocarbons from equipment, machinery, and explosives used.
23	Atmosphere heat	Alterations to local atmospheric heating and terrestrial radiation levels in open-pit mines can vary depending on pit depth, regional geology, and climate.
24	Temperature inversion	Temperature inversions risk trapped air pollution between mine surface and bottom temperatures.
25	Particulate matter	Particulate emissions from diverse sources like drilling, blasting, crushing, and transport operations.
26	Dust	Dust is pervasive due to heavy equipment, blasting, and in-pit crushing common in D&LS mining.
NO	Affecting factor	Definition
27	Air quality	Air quality impacts from mining dust, diesel exhaust, and blasting emissions.
28	Energy demand/consumption	D&LS open-pits require significant energy prompting efficiency improvements and renewable integration to reduce footprints.
29	Clean/Renewable energy generation	Incorporating renewables like solar, wind, geothermal, and hydro aims to lower emissions and fossil fuel dependence in energy-intensive mining.
30	Fossil fuel depletion/ consumption	Heavy trucks rely mostly on fossil fuels to support open-pit operations.
31	Greenhouse Gas Emissions (GHG)	Mechanization and changes to land use, deforestation, and erosion alter carbon cycles and local climates.
32	Carbon Sinks	Destroying carbon sinks exacerbates carbon dioxide increases contributing to climate change.
33	Surface ground's stability/subsidence	Extensive pre-mining disturbance is required, involving vegetation clearing, topsoil and overburden stripping, excavation works, road and infrastructure development, and waste deposition.
34	Slope Stability	At the regional scale, D&LS open-pit mining usually demands sizeable tracts of land undergo alterations through surface clearing and terrestrial excerption practices
35	Land disturbance	Extensive pre-mining disturbance through clearing, soil/overburden removal, excavation, infrastructure development, and waste deposition.
36	Land use	D&LS open-pits usually demand sizeable, altered tracts of land.
37	Reclamation	Extensive clearing, overburden removal, mining, and infrastructure impact landscapes needing reclamation.
38	Landscape & topography	Operations significantly alter topography through excavations and waste piles visible from afar.
39	Fly rock	Fly rock incidents stem from overcharging, poor fragmentation, blasting issues, and timing.
40	Ground Vibration	Ground vibrations impact stability and safety from blasting, machinery, and seismicity.
41	Transport and access roads	Road development benefits and impacts must be weighed at 1000m depths.
42	Geothermal effect	Deeper exposures result in greater subsurface temperatures from natural gradients.
43	Noise	Drilling, blasting, machinery, and crushing generate noise health concerns.
44	Air overpressure	Explosive shockwaves require control and management.

No.	Affecting factor	Definition
1	Production capacity	Mine scale and production capacity are directly tied.
2	Net present value	As capacity rises with scale, mining income will rise.
3	Net profit	As capacity rises with scale, mining profits will rise.
4	Income	As capacity rises with scale, mining income will rise.
5	Mining & plant equipment	IPCC systems need greater capital than trucks and out-of-pit crushers for D&LS open-pit mines.
6	Infrastructures development	D&LS open-pits require considerable capital for automation, mechanization, robotic equipment, and related infrastructure.
7	Construction	D&LS open-pit mines require considerable capital for construction.
8	Recapitalize	D&LS open-pit mines require considerable capital for depreciation costs.
9	Rate of Return	The larger the investment, the longer to return on investment.
10	Drilling and blasting costs	Drilling and blasting costs are directly tied to production capacity, which reflects the mining scale.
11	Loading costs	Loading costs are directly tied to production capacity, which reflects the mining scale.
12	Haulage costs	Haulage costs are significantly dependent on open-pit depth.
13	Primary Crushing costs.	Primary crushing costs are significantly dependent on open-pit depth.
14	Reclamation costs	Rehabilitation costs are directly related to mine depth and scale.
15	Income tax	Large-scale mines pay greater taxes as production capacity is closely associated with income tax.
16	Royalty	Royalty levels are established by legal frameworks and agreements between mines and authorities.
17	Fixed and indirect costs	Fixed and indirect costs are not affected by depth or scale but do affect regional development.
18	Processing, Smelting, refining	Depth or scale does not directly influence processing costs but affects regional development.
19	Gross domestic product	Higher production from a larger scale means a greater contribution to the country's GDP.
NO	Affecting factor	Definition
20	Export	Increased production from a greater scale also increases contribution to national exports.
21	Business opportunities in other sectors	D&LS open-pits require advanced technology and infrastructure leading to other business opportunities.
22	Foreign exchange	
23	Inflation	Exchange rates, inflation, and metal prices are outside miner's control, so depth has no direct impact.
24	Metal/mineral price	
25	Employment rate & duration	Employment rates and durations in D&LS mines lead to varied economic impacts.
26	Poverty generation or reduction	Income generation will affect poverty reduction/generation.
27	Crime generation or prohibition	Economic crimes may increase or decrease.
28	Regional development	Socioeconomic development occurs due to mining activities in a region.

**TABLE 2.** Economic Factors for a Comprehensive Model

No. Affecting factor Definition		
1	Job Satisfaction	Job security and salaries are affected by increased depth and scale.
2	Social Relationship	Mining projects affect family life and community communication.
3	Freedom & Justice	D&LS mines influence freedom and justice in nearby communities.
4	Livability	D&LS mines affect food security, living costs, and communication services.

#### **TABLE 3.** Social Factors for a Comprehensive Model

5	Social Infra & Amenity	D&LS mines develop education, health centers, public services, and leisure activities.
6	Political Stability	Political stability affects investment with a direct relation to social impacts.
7	People's Safety	Communication tools and training for safety assurance are vital in D&LS mines.
8	Equipment Safety	Some equipment used in D&LS open-pit mines are partly different in size, type, and usage and their safety assessment is vital.
9	Material Safety	Materials used in D&LS open-pit mines can be different and their safety assessment is important.
10	Employment	D&LS open-pit mines affect employment/unemployment rates (direct, indirect, local, and national employment).
11	Business Opportunity	D&LS open-pit mines create business opportunities above and underhand.
12	Stakeholders Inclusion	Vital to include stakeholders, especially for D&LS open-pit mine lifetimes.
13	Future Generation Rights	It is important to emphasize the efficient depletion of resources for future generations' rights.
14	Land Ownership & Regin Importance	Land ownership is affected by D&LS open-pit mines, which impacts the region's value.
15	Education	D&LS mines can boost local training and education through new technologies.
16	Equipment & Materials Availability	New technologies and unknown environmental conditions in deep open-pit mines will impact the employment of skilled labor.
17	Human Capital	The availability of skilled, trained, and educated human resources is essential in D&LS open-pit mines.
18	Child/Forced Labor	The inclusion of child labor or forced labor in the mining project has a negative social impact.
19	Health and Safety	Community exposure to physical and mental health issues, fatalities, work-related accidents (failure of structures such as dams), and diseases caused by environmental impacts of the mine.
20	Crimes	Crime in the local community (corruption, bribery, robbery, alcoholism, drugs, domestic, and sexual violence).
21	Demographic Changes	Demographic changes due to mining such as the migration of indigenous people to other regions or the migration of professionals to the mining region.
22	Income Generation & Poverty	Income generation in D&LS open-pit mines can impact poverty (poverty prohibition or generation).
23	Wealth Distribution	The distribution of wealth in mining regions should be fair, to include all stakeholders.
24	Tourism Attraction	Mining projects, specifically D&LS projects, can be a positive tourism attraction if managed in line with SDGs, or reduce tourism attraction if not.
25	Culture	Growing tangible culture (buildings, monuments, landscapes, books, works of art, and artifacts) and intangible culture (folklore, traditions, language, and knowledge) due to the mining project.
26	Legislative Frameworks	The mining project needs to apply the legislative frameworks in the regions.
27	Mining Image	Conflict between indigenous people and mining.

The outcome of this step reveals 44 environmental factors, 28 economic factors, and 27 social factors identified for developing a comprehensive sustainability assessment model, respectively (Tables 1 to 3).

**2.3. SD Indexes Models** Distinct models for three sustainable development (SD) indices were proposed (34-36). The Fuzzy Delphi Analytic Hierarchy Process (FDAHP) technique was used to calculate the importance weight of each factor. To reduce uncertainty in expert judgments and increase the reliability of their responses, Z-numbers were also used along with FDAHP (formula summarized in Table 4). First, the importance weight for each factor group was calculated. Then their scores were found through scenario-based analysis. This process was

repeated for each sustainable development index separately. It resulted in scores for the three distinct SD indexes.

**2. 4. Defining Scenarios** Scenarios can test how sensitive the assessment is to different stakeholders' points of view, by varied weightings given to each index. To capture the complexity of sustainable development in D&LS copper mines, 10 scenarios were created. Each gave a unique set of weights to the environmental, social, and economic dimensions.

The purpose was to thoroughly look at different tradeoffs and priorities of stakeholders. By varying the weights in each scenario, different stakeholder views could be considered. For example, one scenario might emphasize the environment more to minimize ecological harm. Another could weigh social factors higher to focus on community rights and job opportunities. Another could prioritize economics to look at profit, income, and national growth. The defined scenarios capture these varied priorities (Table 5).

Under Equation 12, the final sustainability score for a specific mining site can be determined by multiplying the sustainability score (as shown in Equation 11 in Table 4) of each index by its corresponding weight.

$$S_F = \sum_{n=1}^{3} W_n S_n = \sum_{n=1}^{3} W_n * \left( \sum_{k=1}^{k} W_k * \frac{\sum_{i}^{l} S_{Fi}^*}{j} \right)$$
(12)

$$S_F = \sum_{n=1}^{3} W_n S_n = S_{En} W_{En} + S_{Ec} W_{Ec} + S_{So} W_{So}$$
(13)

where

 $S_n$  is the final sustainability score for the n<sup>th</sup> pillar of SD, calculated by the Z-FDAHP technique,

 $W_n$  is the assigned weight of the n<sup>th</sup> pillar of SD, defined in scenarios,

 $S_{Fj}{}^{\ast}$  is the affecting factor score the  $j^{th}$  factor,

 $W_k$  is the importance weight of the K<sup>th</sup> category, and  $S_{En}$ ,  $S_{Ec}$ , and  $S_{So}$  are the environmental, economic, and social sustainability scores calculated by the Z-FDAHP technique, respectively.

	<b>TABLE 4.</b> Summary of formulas for Z-Fuzzy Delphi AHP (34)			
No.	Equation	Variables definition	Explanation	
(1)	$\alpha = \frac{\int x \mu_{\bar{R}}(x) dx}{\int \mu_{\bar{R}}(x) dx}$	$\mu_{\tilde{R}}(x)$ a triangular membership function	Transforming linguistic Z-numbers to fuzzy triangular numbers	
(2)	$A_{ij} = \left(a_{ij}, \delta_{ij}, \gamma_{ij}\right) * \sqrt{\alpha}$	$\widetilde{A_{ij}}$ the fuzzy representation of the value assigned by experts	Reducing uncertainty of experts' judgments	
(3)	$a_{ij} = Min(\beta_{ijk}), k = 1, 2, \dots, n$	$a_{ij}$ The minimum value of the questionnaires	The 1 <sup>st</sup> component of the fuzzy number $\widetilde{A_{ij}}$	
(4)	$\delta_{ij} = \left(\prod_{k=1}^n \beta_{ijk}\right)^{\frac{1}{n}}, k = 1, 2, \dots, n$	$\beta_{ijk}$ The relative importance of factor i on factor j from the expert's viewpoint k	The second component of the fuzzy number $\widetilde{A_{ij}}$	
(5)	$\gamma_{ij} = Max(\beta_{ijk}), k = 1, 2,, n$	$\gamma_{ij}$ The maximum value of the questionnaires	The third component of the fuzzy number $\widetilde{A_{\iota J}}$	
(6)	$\tilde{A} = \begin{bmatrix} \tilde{a}_{ij} \end{bmatrix}$ $\widetilde{a_{ij}} \times \widetilde{a_{ij}} \approx 1, \forall i, j = 1, 2,, n$	$\tilde{A}$ The fuzzy positive reciprocal matrix between the various factors	The different factors' fuzzy positive reciprocal matrix	
(7)	$\tilde{Z}_{i} = \left[\tilde{a}_{ij} \otimes \otimes \tilde{a}_{in}\right]^{\frac{1}{n}}$	$\tilde{Z}_i$ The relative fuzzy weight of the factors	The relative fuzzy weight of the factors	
(8)	$\widetilde{W}_i = \widetilde{Z}_i \otimes [\widetilde{Z}_i \oplus \ \oplus \widetilde{Z}_n]^{-1}$	$\widetilde{W}_i$ Fuzzy weight of the ith factor.	$\widetilde{W_t}$ is a row vector that contains a fuzzy weight for the i <sup>th</sup> factor	
(9)	$W_i = \left(\prod_{i=1}^3 w_{ij}\right)^{\frac{1}{3}}$	$W_i$ Weight of factor i.	The defuzzification formula	
(10)	$S_k = \frac{\sum_{1}^{j} S_{Fj}^*}{j}$	$S_k$ is the final score of the $K^{th}$ category $S_{Fj}{}^*$ is the affecting factor score the $j^{th}$ factor	Scoring the affecting factors	
(11)	$S_n = \sum_{k=1}^k W_k S_k$	$W_k$ is the importance weight of the K <sup>th</sup> category $S_n$ the sustainability score for each SD index	Sustainability Score (S <sub>n</sub> )	

 TABLE 5. Different scenarios for SD index weights

Scenario No	WEnvironment	WEconomic	W <sub>Social</sub>
Base Model (Scenario 1)	0.33	0.33	0.33
Scenario 2	1	0	0
Scenario 3	0.6	0.2	0.2
Scenario 4	0.2	0.4	0.4
Scenario 5	0	1	0
Scenario 6	0.2	0.6	0.2
Scenario 7	0.4	0.2	0.4
Scenario 8	0	0	1
Scenario 9	0.2	0.2	0.6
Scenario 10	0.4	0.4	0.2

The final sustainability score ranges from 0 to 10. This shows how well a mine meets its environmental, economic, and social duties to stakeholders.

A score of 10 means full sustainability - the mine handles all three SD indexes very well.

A score of 0 means unsustainability in all three parts. It shows the mine is not managing the environmental, economic, or social aspects properly.

#### **3. VERIFICATION**

The Sungun Copper Mine (SCM) in northwest Iran is the second largest copper mine in the region, with the Sarcheshmeh copper mine in the southeast being the largest. It is globally renowned for its large copper deposits, with a total ore reserve of approximately 1.2 billion tons and an average copper grade of 0.67% (see Figure 2). The mine design specifies that the final pit top will have a maximum width of 1.7 km and a minimum width of 1.2 km. The Ultimate Pit Limit (UPL) is anticipated to be at an altitude of 1,400 meters above sea level, resulting in an ultimate pit depth of approximately 900 meters (36).

To evaluate and benchmark the sustainability performance of SCM, a sustainability assessment model has been applied. Previous studies conducted by the authors have determined "the environmental, economic, and social sustainability scores of SCM to be 3.326, 5.298, and 6.364, respectively. By applying 10 different scenarios defined in Table 5, the sustainability score of the SCM mine can be determined under each scenario, using Equation 12.

#### 4. RESULTS

The model applied the 10 scenarios in Table 5 using Equation 12 to determine SCM's final sustainability score. The highest score was achieved under scenario 8, where social factors received the highest weight of 1. This suggests social indicators strongly influence SCM's sustainability performance. Aspects like community impacts and worker conditions are important considerations for long-term sustainable operations. Focusing only on the economic viability of a mining project may overlook these dimensions.

The lowest score was under scenario 2, relying solely on environmental indicators. This implies SCM is not paying enough attention to the environmental impacts of the mining activity.

The highest and lowest scoring scenarios likely show how sensitive the overall results are to how sustainability dimensions are weighted. Valid perspectives exist beyond any single weighting approach.



Figure 2. SCM's geographical location (34)

Table 6 shows the score calculations for each scenario. Tables 7 and Figure 3 present the final scores for all ten scenarios.

**TABLE 6.** Calculations for each scenario (On a scale of 0-10)

Scenario	Calculation	
Base Model (Scenario 1)	$\begin{split} S_F &= \sum_{n=1}^{3} W_n S_n = S_{En} W_{En} + \\ S_{Ec} W_{Ec} + S_{So} W_{So} = 3.326 * 0.33 + \\ 2.111 * 0.33 + 6.364 * 0.33 = 3.894 \end{split}$	3.894
Scenario 2	$S_F = 3.326 * 1 + 2.111 * 0 + 6.364 * 0 = 3.326$	3.326
Scenario 3	$S_F = 3.326 * 0.6 + 2.111 * 0.2 + 6.364 * 0.2 = 3.691$	3.691
Scenario 4	$S_F = 3.326 * 0.2 + 2.111 * 0.4 + 6.364 * 0.4 = 4.055$	4.055
Scenario 5	$S_F = 3.326 * 0 + 2.111 * 1 + 6.364 * 0 = 2.111$	2.111
Scenario 6	$S_F = 3.326 * 0.2 + 2.111 * 0.6 + 6.364 * 0.2 = 3.205$	3.205
Scenario 7	$S_F = 3.326 * 0.4 + 2.111 * 0.2 + 6.364 * 0.4 = 4.298$	4.298
Scenario 8	$S_F = 3.326 * 0 + 2.111 * 0 + 6.364 *$ 1 = 6.364	6.364
Scenario 9	$S_F = 3.326 * 0.2 + 2.111 * 0.2 + 6.364 * 0.6 = 4.906$	4.906
Scenario 10	$S_F = 3.326 * 0.4 + 2.111 * 0.4 + 6.364 * 0.2 = 3.448$	3.448

**TABLE 7.** Final sustainability score for each scenario (On a scale of 0-10)

Sustainability Indexes' scores		Environment	Economic	Social	Final Sustainability Score
		3.326	5.298	6.364	01
	Base Model (Scenario 1)	0.33	0.33	0.33	4.946
ghts	Scenario 2	1	0	0	3.326
Weig	Scenario 3	0.6	0.2	0.2	4.328
cs,	Scenario 4	0.2	0.4	0"4	5.330
ndex	Scenario 5	0	1	0	5.298
lity I	Scenario 6	0.2	0.6	0.2	5.117
inabi	Scenario 7	0.4	0.2	0.4	4.936
ustai	Scenario 8	0	0	1	6.364
Ø	Scenario 9	0.2	0.2	0.6	5.543
	Scenario 10	0.4	0.4	0.2	4.722



Figure 3. Final sustainability score for each scenario

#### **5. DISCUSSION**

The sustainability assessment model was applied to determine the Sungun Copper Mine's (SCM) final sustainability score. SCM is a D&LS open-pit mine in northwest Iran. The results show SCM's sustainability depends on the weights given to environmental, social, and economic factors, from different stakeholders' perspectives.

D&LS open-pit mines can generate long-lasting environmental impacts by stripping away large areas of land and disposing of huge amounts of waste rock and tailings. Surface and groundwater quality may be greatly lowered from acid mine drainage. Greenhouse gas emissions are also high due to energy-intensive mining and materials movement. Irreparable damage to ecosystems and biodiversity may occur without mitigation measures.

At SCM specifically, deforestation of the Arasbaran region could be a concern. Mitigation plans should minimize the project's footprint in forest areas as much as possible to limit habitat loss. Creating new habitats may be needed. Rehabilitation of disturbed forest zones could help accelerate the recovery of this ecosystem since revegetation timelines exceed the mine's lifespan. Priority rehabilitation could help speed up forest recovery.

Economic viability is also important for sustainability. D&LS open-pit mines require massive upfront costs and finances to justify expenses. Financial stability ensures ongoing local jobs and benefits as mining progresses deeper. Neglecting economics risks project cancellation due to a lack of profits, disputes, or funding access.

Prioritizing only social factors also threatens to undermine trust in companies over time. Communities and markets increasingly demand responsibility across all aspects of sustainability.

The mine scored lowest under scenario 2 where only the environment mattered. But exclusively focusing on environmental protection is problematic for major openpit mines too. It could make projects uneconomical or impose constraints making the core business unviable, without considering economic and social trade-offs. Ignoring economics risks financial instability. Uncontrolled rising costs from unrealistic environmental demands could force early closure. Similarly, dismissing social issues ignores communities near major environmental disruptions. Failing to address social impacts could weaken acceptance over time. This implies that to gain SDG in D&LS open-pit mines, a balanced approach is needed. Rather than favor any single sustainability factor, sustainable development at SCM requires adaptive, integrated strategies that find the right balance between environmental, economic, and social impacts over the long run through close collaboration with stakeholders. This balance can be achieved through scenarios 9, 4, and 6 with scores of 5.543, 5.330, and 5.117 out of 10, respectively.

Deep and Large-scale open-pit mines like SCM present unique difficulties due to their extensive excavation, potential harm to the environment, and social consequences. The proposed model offers an effective way to address these challenges. By including economic, environmental, and social aspects, the final sustainability model in this study understands the complexity of these mining operations and encourages balanced decision-making.

The model examines a wide range of 99 indicators as sustainability measures. This broad examination gives a comprehensive look at how the mine is doing across multiple areas, including issues specific to D&LS openpit mines.

The Z-FDAHP technique used to calculate importance weights for the sustainability indicators deals with the natural uncertainties and biases involved in assessing sustainability, especially for complex mines. It allows expert input and consensus building, leading to more reliable weights.

The model also analyzes scenarios to assess sustainability performance from different stakeholders' perspectives, under various weightings assigned to each sustainability index. This recognizes sustainability frequently changes as priorities and stakeholder views differ. Looking at different scenarios provides a greater understanding of the relative significance of environmental, social, and economic aspects for sustainable development at these mines. It is important to consider the intended audience of the sustainability report and their particular priorities. The recipient may place more emphasis on some factors over others. Evaluating scenarios allows for a more nuanced analysis that accounts for the end user's perspective. This consideration of the target audience is an important but

often overlooked part of environmental impact assessments and sustainability evaluations in previous related studies. Considering who will receive the findings and what matters most to them enhances the relevance and usefulness of the analysis.

The results of this study provide a valuable understanding of prioritizing environmental, social, and economic aspects in D&LS open-pit mines to identify the most sustainable practices under different conditions. This can encourage sustainable practices in mining and help meet sustainable development goals.

#### 6. CONCLUSION

This study developed a comprehensive sustainability assessment model and validated it through application to the Sungun Copper Mine case study. The model takes a holistic, multi-dimensional approach to evaluate mining projects across a wide range of 99 environmental, social, and economic indicators. Its scenario-based structure allows customization based on project contexts and stakeholder perspectives.

Application of the model to Sungun Copper Mine demonstrated its functionality and provided valuable insights into priority issues. Examining varied scenarios highlighted the importance of tailoring assessments based on audience. The results also showed the need for balanced consideration of all sustainability factors. Engaging stakeholders in the application process helps ensure assessments remain grounded in operational realities. Integration of outputs into sustainability strategies and programs supports focused action.

The model incorporates the 99 factors using Z-FDAHP and offers a formula to calculate sustainability scores under scenarios. This tool allows stakeholders to assess adherence to responsible practices. Quantifying performance provides a transparent and measurable representation aligned with sustainability goals. This enhances stakeholder involvement and decision-making.

Considering diverse aspects of sustainable development across multiple scenarios strengthens the model's usefulness across mining contexts. The model fills gaps in knowledge by taking a comprehensive approach tailored to this context.

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#### Persian Abstract

معادن روباز عمیق و بزرگ مقیاس (D&LS) می توانند اثرات مختلف محیط زیستی، اجتماعی و اقتصادی بر ذینفعان و جوامع محلی، منطقهای، ملی و بینالمللی داشته باشند. شناسایی این اثرات و داشتن مدل جامعی برای ارزیابی همزمان آنها برای دستیابی به اهداف توسعه پایدار (SD) حیاتی است. در این مطالعه یک مدل ارزیابی پایداری ارائه شده است که شامل ۹۹ عامل تأثیر در بعدهای محیط زیستی، اجتماعی و اقتصادی است. امتیاز پایداری با استفاده از تکنیک FDAHP محاسب شد تا قضاوت شخصی و عدم قطعیت در نظرات متخصصان کاهش یابد. سپس از تکنیک مبتنی بر سناریو برای لحاظ کردن دیدگاههای ذینفعان مختلف در مدل استفاده شد. این مدل در معدن مس سونگون در شمال غربی ایران پیاده شد. نتایج نشان داد که عملکرد پایداری معدن مس سونگون حساسیت بسیار بالایی نسبت به وزندهی شاخصها دارد. بالاترین امتیاز پایداری با تاکید بر شاخص اجتماعی (امتیاز پایداری کمتری داشته و نتایج آن به ترتیب ۳۳۲۲ و ۸۲۵۹ بود. رویکرد مبتنی بر در نظرگرفتن همزمان سه شاخص توسعه پایدار با ساخی محیطی یا اقتصادی، امتیاز پایداری کمتری داشته و نتایج آن به ترتیب ۳۳۲۲ و ۸۲۵۹ بود. رویکرد مبتنی بر در نظرگرفتن همزمان سه شاخص توسعه پایدار با همکاری ذینفعان به معنای اجرای همزمان سه شاخص توسعه پایدار است که توسط امتیازات پایداری ۵۵٬۰۰۵ و ۲۰۱۵ و ۲۰۱۵ و ۲۰۱۵ و ۲۰۱۵ و ۲۰ ارزیابی پایداری ارائه شده، اطلاعات باارزشی را برای شرکتهای معدنی و ذینفعان فراهم می در ساز معدنی معر فرمان سه شاخص توسعه پایدار با همکاری ذینفعان ارزیابی پایداری ارائه شده، اطلاعات باارزشی را برای شرکتهای معدنی و ذینفعان فراهم می کند تا بهتر بوژه همید تا بهتر بتوانند تاثیرات پروژه معدنی، متیر بوژه می می و بررگ مقیاس را بر ابعاد مختلف توسعه پایدار ارزیابی کند. مدل پایداری ۲۵۵/۱۵ و ۲۰۱۰ و در سازه در سازیوهای ۸۳ و می از خصامی و بوز عمیق و بزرگ مقیاس را بر ابعاد مختلف توسعه پایدار ارزیابی کند. مدل پریتی و دی نفعان به مر می کند تا بهتر بوژه می معدنی، بالاخص می و اور عمیق و بزرگ مقیاس را بر ابعاد مختلف توسعه پایدار ارزیابی کند. مدل پایداری شده به دلیل به کارگیری مجموعه جامع ۹۹ عمل محیط زیستی اختماعی و اقتصادی، توانایی در نظرگرفتن اوزان متفاوت برای شاخصها در سازیوهای مختلف بر اساس دیدگاه ذینفعان؛ و اعتبارسنجی با استفاده از می موردی، رویکردی جدید و نوآورانه ارانه داده. ا

چکيده



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## Development of a Novel Super-active Ziegler-Natta Polyethylene Catalyst: Study on Structure, Performance and Application

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#### PAPER INFO

#### ABSTRACT

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Keywords: Polyethylene Pipes Malvern Super-active Catalyst-510 Ziegler-Natta Catalysts In this research, the synthesis process of a novel super-active catalyst, named SAC-510 is investigated at experimental scale. The authors compared the analyzed data against those derived from a popular catalyst, *Finix-112*, and several other available alternatives. The data indicated that SAC-510 catalyst derived the optimal activity from its spherical particles. Titanium and other chemical elements were less uniformly distributed in SAC-510 than in *Finix-112* samples, with the mean particle size being slightly larger than that found in *Finix-112*. The pores' dispersion and sizes in SAC-510 were not as uniformly distributed as those in *Finix-112* catalyst. Lastly, both SAC-510 and *Finix-112* catalysts were equally adaptable for use in high-density polyethylene pipes (grade 100). Compared to other commercially available catalysts, the major advantages of SAC-510 are the economical use of hydrogen and monomers, and low purging of its valuable gases during the polymerization process. The results obtained are as follows: the increase in oxidative induction time efficiency with SAC catalyst compared to Finix catalyst by 5.8%, activity by 35.7%, hydrogen responsibility by 24.39%, 1-butene consumption by 8.38% and triethylaluminium consumption by 27.27%.

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NOMENCLATURE				
SAC-510	Super active catalyst	d	Diameter	
PSD	Particle size distribution	DSC	Differential Scanning Calorimeter	
OIT	Oxidation Induction Time	$V_p$	Pore volume	
GPC	Gel permeation chromatography	$r_p$	Pore peak radius	
HDPE	High density polyethylene	$a_p$	Specific pore area	
PE100	Polyethylene pipe grade of 100	Greek Symbols		
SEM	Scanning electron microscopy	μ	Micron	

#### **1. INTRODUCTION**

Society, in general, and the industry, in particular, have significantly included plastics for changing different materials. High density polyethylene (HDPE) is a semicrystalline polymer widely used for the transport of drinking water supplies (1, 2). These are often exposed to different weathering conditions, for example in outdoor applications or when the freshly extruded pipes are stored in the open before their installation (3). Polyethylene (PE) is known as one of the most commonly-employed thermoplastic polymer, which have demonstrated its brilliant advantages in different industrial-based activities like wires/cables insulation, agricultural mulch, membrane-based gas separation and medical engineering due to its ease of installation, absence of corrosionrelated problems, low cost and projected 50 to 100-year service life (4-6). Ziegler-Natta catalyst is a commonlyused catalyst in a bimodal slurry system for HDPE production. This promising catalyst is made based on the mixture of different chemical components that are prominently applied in the synthesis process of 1-alkenes

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polymers (i.e., alpha-olefins) (7, 8). Titanium, and to a lesser extent, chrome and vanadium are regarded as important metallic elements in Ziegler-Natta catalysts (9). They have enabled scientists to polymerize many organic compounds, such as alkenes and dienes with superior activity and selectivity, under a wide variety of experimental conditions. Since their advent, these catalysts have also played a significant role in the development of valuable products, highly needed in petrochemical and plastic industries (9). In this context, the role of titanium and magnesium is particularly well known in the production and use of polyethylene products (10). Currently, scientists are conducting much research with a focus on the activity, particle morphology and distribution, hydrogen response, and performance of catalysts and co-catalysts (11-13).

Among the commonly-applied polymerization processes, ethylene slurry has attracted much scientific attention. In addition to improving the activity of catalysts, controlling the particle size and its distribution in polyethylene products are of significant importance (14-17). In the recent published research articles, various aspects of catalysts and their interactions with cocatalysts and intermediate metals have been investigated. These include, *a*) controlling titanium oxidation; *b*) effect of external and internal donors (18, 19); c) the role of cocatalysts (20); d) effect of newly developed catalysts (21, 22); and, e) synthetic and modelling studies in the polymerization field (23-26). In addition to the molecular structures of catalysts, the polymerization and industrial process have an essential role in the production of polymers with a variety of properties, and promoting scientific research on these products (27-30). During 1980's and 1990's, a series of patented methods on the preparation of new Ziegler-Natta catalysts has been introduced (31, 32). Later studies proposed and examined the role of titanium alkoxide to replace the use of Titanium tetrachloride (TiCl<sub>4</sub>). In these products at least one alkoxide ligand connects Ti (OR) 4 to tetra-titanium alkoxide. A good example of this subject is the polymerization of olefin compounds (33-35).

To introduce a wide range of molecular weights in manufacturing resins, Ziegler-Natta catalysts require different reactors that operate under specific conditions of temperature, monomers, and hydrogen concentration, used in series or singly, which involve high costs (17, 36-38). In this context, there exists an urgent need for new catalysts with better performance to produce bimodal resins with added market value. For this purpose, two methods are popular for the preparation of the main components of the catalyst. The first method involves a solid carrier, consisting of a magnesium dihalide reaction with titanium or vanadium in a suspended hexane environment. This method provides the components of the catalyst, although it is difficult to control the polyethylene product, the particle size, and its distribution (39). In the second method, a magnesium compound, such as magnesium dichloride, is dissolved in a solvent, so that homogeneous solid particles of magnesium or titanium precipitate after adding a titanium compound. This process can provide the main component of the catalyst upon its solid processing with another liquid titanium compound and a co-catalyst (40).

This study aims to synthesize and manufacture a novel and efficient super-active Ziegler-Natta catalyst, named *SAC-510* toward the production of a new generation of high-density polyethylene pipes. Subsequently, the authors analyzed the particle morphology and its performance, compared to a popular catalyst, *Finix-112*, and several other commercially available alternatives. We have obtained some promising results, which are presented and discussed in the present article.

#### 2. MATERIALS AND METHODS

**2. 1. Materials** All of the materials for the polymerization processes of both the support catalyst, and the final super-active catalyst (SAC-510) were obtained from the Shazand Petrochemical Technology Company (Arak, Iran) and Pooyesh Co. (Tehran, Iran). Hexane (C6H14) was utilized as the solvent and copolymerization agent. Ethylene was used as the main feed for the polymerization process. Lastly, 1- butylene and hydrogen were used as the components required for the polymerization. Triethylaluminium (97%) was purchased from Fluka Chemie GmbH (Buchs, Switzerland). Oxygen 4.5 (purity 99.995%) and nitrogen 5.0 (99.999% purity) were obtained from the Shazand Petrochemical company.

#### 2.2. Equipment

**2.2.1. Glove Box** To store and preserve the catalysts and co-catalysts in this study, we used a glove box unit (Cleatech; Orange, CA, USA). This unit prevented the active sites in catalysts and sensitive chemicals from getting contaminated and oxidized, under a nitrogen atmosphere.

**2. 2. 2. Scanning Electron Microscopy/ Energy Dispersive X-ray Analysis (SEM/EDX)** The surface morphology of the catalyst was examined by Scanning Electron Microscope (SEM) (model JSM-5910, JEOL Inc., Peabody, MA, USA) under high vacuum microprobe. This microscope provided scanned images, analyzed the X-ray emitted from the particles, and determined the accurate weight and percentage of the elements contained in the samples [40].

**2.2.3. Malvern Analyzer** In addition to the SEM analysis, the particle sizes and molecules contained in the

samples were also measured on a Malvern analyzer (Entegris; Dresden, Germany). The images obtained from this analyzer were based on the principle of dynamic light scattering.

**2.2.4 Buchi Reactor** Made of stainless steel with a volume of 1 liter is used for slurry polymerization. The volume of the reactor jacket is 300ml. Addition of catalyst and co-catalyst is by injection under pressure.

**2. 2. 5. Gel Permeation Chromatography (GPC)** To analyze the different particle species of large molecular sizes, such as polymers, we measured the particle's molecular weights on a gel permeation chromatography unit (GPC-150-II+IR5; Cambridge Polymer Group, Inc.; Woburn, MA, USA) (41).

**2. 2. 6. Differential Scanning Calorimeter (DSC)** The objective of the test is to represent the duration in time of the heat stabilizer until its deterioration through oxygen and heat. The period of time from the switching over to oxygen until the onset of the oxidation reaction (point of intersection of the basis line with the tangent) is referred to as the induction period (Oxidation Induction Time, OIT). A long induction period shows good stabilization and vice versa. The described test method is carried out in dependence on DIN EN728 and we used Differential Scanning Calorimeter unit (Mettler-Toledo DSC 822e.) (42).

**2. 2. 7. Huber Circulator** We utilized a Huber circulating bath (Ministat CC3 Huber UK; Derbyshire, UK) to control the temperature within the reactor's jacket, ranging from -50 °C to +350 °C.

#### 2.3. Methods

**2. 3. 1. Preparation and Polymerization** The methods for the polymerization processes, as established by earlier studies (39, 40, 43).

2. 3. 1. 1. Magnesium Ethoxide Powder This material was necessary to make the base product. The construction of super active Ziegler-Natta catalysts for ethylene polymerization requires substrates for the stability of the active centers of the catalyst. Metal halides and oxides have been proposed as suitable bases for catalysts, and in the meantime, magnesium ethoxide is very suitable for making the super active Ziegler-Natta catalyst. To prepare the super active catalyst base, commercial magnesium ethoxide (Mg(OC<sub>2</sub>H<sub>5</sub>)) is first prepared in pure form with the conditions presented in Table 1. The average particle diameter of the primary magnesium ethoxide powder is 500 microns, so that more than 90% of the particles have a diameter in the range of 200 microns to 1200 microns. Titanium sits better on the substrate when the size of the primary powder particles is reduced and their distribution is uniform. Magnesium ethoxide with a diameter of about 500 microns forms a suspension in an inert saturated hydrocarbon after mechanical crushing by a jet mill to a size of about 8 microns using a Jet pulverizer (Jet Mills; Moorestown, NJ, USA). Table 1 presents aims to present different features of the magnesium ethoxide for the catalyst bed.

2. 3. 1. 2. Magnesium Ethoxide Suspension Gel The magnesium ethoxide powder was then suspended in a neutral, aliphatic hydrocarbon until the mixture was ready to convert into gel. Ideal hydrocarbons for this purpose are butane, hexane, cyclohexane, heptane, isooctane, and several others including toluene and xylene. Also, hydrogenated oils devoid of oxygen and sulphur would be appropriate. About 200 grams of the sample is taken under  $N_2$  atmosphere and injected into a 5-liter reactor containing two liters of hexane. Then carbon tetrachloride is added and after mixing(100rpm), the temperature of the reactor is increased to about 60 degrees, and this process is allowed to continue for 24 hours. In this case, the solvent penetrates into the crystal layers and causes the particles to take a gel-like shape. If the gelling process has progressed correctly, after stopping the mixer, it takes about 30 minutes for the particles to settle.

Injecting 7 ml of titanium tetrachloride into the gel produced at 80 degrees Celsius to place titanium on the gel bed.

**2. 3. 1. 3. Catalyst Assisted Preactivation** The choice of co-catalyst has a great influence on the performance of titanium-based Ziegler Nata catalysts. Catalyst assistance affects activity, molecular weight and molecular weight distribution. By increasing the amount of catalyst aid, the activity of all active centers decreases to almost one level. In order to produce active sites, which Mr. Kissin divided into five types by fluorescent distribution, the catalyst must be placed in the vicinity of triethyl aluminum (TEA) for a certain period of time.

**2. 3. 1. 4. Determination Of The Catalyst Content** A 10ml aliquot of the catalyst was removed from its container, using a syringe, and poured in a small glass dish with known weight. After the sample was cooled

**TABLE 1.** Strouhal number for different geometric cases

Magnesium Species	Percentage of Total Weight
Total magnesium content	21-22%
Total Mg (OH) <sub>2</sub> & MgCO <sub>3</sub> contents	<1%
Total C <sub>2</sub> H <sub>5</sub> OH content	<0.3%

down, the weight of the empty dish is deducted from the total weight of the dish containing the catalyst 10ml aliquot. The net weight of the catalyst sample varies depending on the solvents, such as hexane, used for the polymerization processes.

2.3.1.5. Polymerization Prior to this step, the reactor was purged by running nitrogen ( $\leq 0.1$  bar) through it at 100°C for 60 minutes. Subsequently, the oil circulator pump of the reactor was set at 4500 rpm, and the temperature reset to 60°C. At this temperature, the reactor was cleared with ethylene gas three times at 3-bar pressure. Then, 500 ml hexane at 0.1 bar, and 400 mg/ml triethylaluminium (TEAL) were injected into the reactor and the agitator turned on at 200 rpm. The TEAL was mainly used for the purpose of removing contaminations from the solvent and activation of sites in the catalyst. After 30 minutes from the injection of TEAL, 1-butylene was injected to the reactor at a set amount, and allowed to mix with TEAL and the solvent for 15 minutes with the agitator set at 200rpm. During a 30-min preactivation time, the concentration of catalyst diluted in hexane reached 2mg/ml.

After determining the reactor's pressure at optimal temperature, the catalyst was injected in the reactor under pressure. Next, the reactor's software program was set to reaction mode and the polymerization synthesis plots being printed. During this process, the reaction temperature was closely monitored at 83°C (±1°C) while ethylene was being injected into the reactor at 8 bar. The estimated time for the polymerization of ethylene with 1butylene in the presence of the catalyst SAC-510 was approximately 180 minutes. At the completion of this final step, the reactor's software program was set to "Reaction Off". This terminated the ethylene entry into the reactor and the circulator's temperature was set at 60°C. After the reactor cooled down, the lid was opened, the chamber was cleaned thoroughly with nitrogen, and the catalyst and solvents residues were wiped out.

**2.3.2. Surface Area Analysis (SSA)** The surface area and pore size analysis of the catalyst were carried out by Surface Area Analyzer (Quanta chrome Nova Station A), using nitrogen adsorption method. The sample was initially degassed at 200 °C for 4 h. Surface area of the catalysts was calculated from the nitrogen adsorption isotherm data, using Brunauer, Emmett and Teller (BET) equation. The pore size and pore volume of the catalysts were calculated from N<sub>2</sub> adsorption isotherm data with the help of Barrett, Joyner, Halenda (BJH) model (44).

#### 3. RESULTS AND DISCUSSION

3. 1. Particles Morphology

Understanding the

morphology of micro particles can assist us predict their mass transfer and heat as they go through polymerization processes (45). Initially, monomers penetrate into the catalyst's pores and start numerous active reaction sites, forming the basic polymer particles and clumps as they combine with the catalyst and continue to grow. Later, layers of the polymer are deposited on the catalyst's spherical macro particles, leading to the final polymerized product. Thus, examining the particles reflects the true physical nature of the combined polymer and catalyst (46). Results from this study's tests and experiments are presented below followed by the pertinent discussion under each subsection.

#### 3. 2. Energy Distribution Analyses of the Catalysts'

**Powders** Table 2 represents the results of energy distribution in the two powdered catalysts, *Finix-112* and *SAC-510*, under scanning X-ray analysis (SEM-EDXA). As shown in Table 2, four and three zones were examined, respectively, under SEM-EDXA using the powdered samples of *Finix-112* and *SAC-510* catalysts. The results indicated that there were relatively uniform percentages of the chemical elements, especially titanium, in the *Finix-112* samples. However, much less uniformity was observed in the *SAC-510* samples. Figure 1 shows the electron microscopic images of powdered *Finix-112* and *SAC-510* catalysts, and the differences in the distribution of the particles for both samples.

Evidently, the differences in the percentage and uniformity of the elemental distributions in both catalysts' samples arise from their chemical nature and formulation. Based on the images illustrated in Figure 1, it is perceived that the presence of smaller catalyst particles makes the mobility of larger particles easier, thereby facilitates the polymerization reaction. A major advantage of SEM-EDXA is its better capability of determining the compositional elements in powdered catalysts than that achieved by either XRF or ICP method. The SEM-EDXA method is able to recognize such elements as oxygen, carbon and halogen. Also, it

**TABLE 2.** Scanning electron microscopic features of the Finix-112 and SAC-510 powders

Finix-112	Ti	Mg	Cl	Al	0	Cu	Si
EDAX-1	4.94	20.98	35.85	0.49	37.32	0.42	-
EDAX-2	3.37	14.17	36.06	0.34	45.72	0.38	-
EDAX-3	3.79	15.7	39.28	0.36	40.60	0.28	-
EDAX-4	4.36	13.3	44.70	0.09	36.77	0.51	-
SAC-510	Ti	Mg	Cl	Al	0	Cu	Si
EDAX-1	8.01	14.45	42.36	1.82	30.99	1.47	0.89
EDAX-2	5.48	17.44	28.01	3.29	42.79	0.73	2.25
EDAX-3	6.25	18.51	32.21	3.4	35.64	0.76	2.24



**Figure 1.** Scanning electron microscopic images of the catalysts Sac-510 and Finix-112 powders.a,b) SEM MAG=1 kx, 50µm; c,d) MAG=2.5kx, 20µm; e,f) SEM=1kx,50µm

provides the distribution patterns and variations in the concentration of elements in different areas of various samples at large magnification.

#### 3.2. Particle Size Distribution - Malvern's Method

Figure 2 represents the particles' volume of distribution and their sizes in the micron scale for both catalysts, based on Malvern's method. As seen in Figure 2, the particles in both catalysts occurred similarly in one uniform population each (range: 2-11  $\mu$ m vs 3-30  $\mu$ m). The single peak (50%) for Finix-112 catalyst occurred approximately at 6.8 $\mu$  while that of SAC-510 was about 8.6  $\mu$ m. The data for the particle size distribution in both groups of catalysts are summarized in listed in Tables 3 and 4.

The data in Tables 3 and 4 indicate that the average particle size for SAC-510 catalyst was slightly larger than that of Finix-112. In this context, 10% of the SAC-510



Figure 2. Particle size distribution of SAC-510 (super active) and Finix-112 catalysts

	Size (µm)	Vol Under %										
	2	8.97	16	97.77	45	100	128	100	345	100	850	100
	3	11.39	17	98.55	50	100	132	100	370	100	898	100
	4	17.81	18	99.09	52	100	142	100	385	100	950	100
	5	28.31	19	99.45	54.3	100	160	100	400	100	1000	100
	6	40.66	20.5	99.77	58.5	100	168	100	450	100	1125	100
2	7	52.83	22.3	99.91	63	100	177	100	500	100	1250	100
ζ-115	8	63.66	24	99.98	68	100	190	100	525	100	1325	100
CINI	9	72.69	26	100	73	100	205	100	550	100	1400	100
Ц	10	79.9	28	100	76.5	100	227	100	575	100	1500	100
	11	85.46	30.2	100	80	100	250	100	600	100	1600	100
	12	89.66	32	100	89	100	262	100	634	100	1740	100
	13	92.76	34.8	100	98.2	100	275	100	668	100	1880	100
	14	95.02	37	100	111	100	297	100	735	100		
	15	96.63	40.5	100	125	100	320	100	800	100		

**TABLE 3.** Particle size distribution in Finix-112 and SAC-510 catalysts

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	Size (µm)	Vol Under %										
	2	4	16	89.6	45	100	128	100	345	100	850	100
	3	6.25	17	91.8	50	100	132	100	370	100	898	100
	4	10.42	18	93.56	52	100	142	100	385	100	950	100
	5	17.19	19	94.97	54.3	100	160	100	400	100	1000	100
	6	25.86	20.5	96.56	58.5	100	168	100	450	100	1125	100
	7	35.38	22.3	97.86	63	100	177	100	500	100	1250	100
-510	8	44.87	24	98.66	68	100	190	100	525	100	1325	100
SAC	9	53.76	26	99.26	73	100	205	100	550	100	1400	100
	10	61.72	28	99.6	76.5	100	227	100	575	100	1500	100
	11	68.64	30.2	99.82	80	100	250	100	600	100	1600	100
	12	74.53	32	99.91	89	100	262	100	634	100	1740	100
	13	79.46	34.8	99.97	98.2	100	275	100	668	100	1880	100
	14	83.54	37	99.99	111	100	297	100	735	100		
	15	86.89	40.5	100	125	100	320	100	800	100		

**TABLE 4.** Particle distribution in the catalysts based on

 Malvern method

Catalyst	SAC-510	Finix-112
D (0.1)	3.9µm	2.5µm
D (0.5)	8.6µm	6.8µm
D (0.9)	16.2µm	12.1µm

particles fell within 3.9  $\mu$ m in size while the same percentage of Finix-112 particles had a 2.5  $\mu$ m size. Further, about 90% of the particles in SAC-510 group had a size of 16.2  $\mu$ m while those in Finix-112 group were about 12.1  $\mu$ m in size.

The mechanical measurement of catalysts' particle size and their distribution are performed broadly in industries, which is a critical parameter for manufacturing numerous products. In this respect, Malvern is a highly accurate method for measuring particle sizes ranging from low nanometer to several millimeters.

**3.3. BET Test** Using the popular (BET) test (23), we analyzed the features and dimensions of the pores in both Finix-112 and SAC-510 catalysts. The data from this analysis are presented in Table 5.

**TABLE 5.** Results of the SAC-510 and Finix-112 powders based on BET test

Property	SAC-510	Finix-112
Specific area (m <sup>2</sup> /g)	22.492	24.759
Total Pore volume (cm <sup>3</sup> /g)	0.1746	0.1213
Average pore dimension (nm)	31.051	19.592

The overall results obtained from BET test revealed that the specific area for the pores in SAC-510 was 9% less than that of Finix-112. Also, the mean dimension and volume of the pores in SAC-510 catalyst were greater than those determined for Finix-112 catalyst.

Considering the above data, it can be argued that the dimensional features of the porosity in SAC-510, compared to those in Finix-112, decreases the ability of this catalyst to respond to physical forces. Also, it is likely that larger pores may be deeper in SAC-510 with smaller lateral surfaces, which further contribute to its lower tolerance against shocks, vibrations and other destructive forces.

**3. 4. Barrett-Joyner-Halenda Test** Also, we used another popular test, Barrett-Joyner-Halenda (BJH), to determine the volume and distribution of pores in the catalysts (23). The data from our BJH test on both catalysts are presented in Table 6. Specifically, Table 6 reflects accurate information about three important variables for each of the two catalysts: a), the pore volume (Vp); b) the pore peak radius (rp); and c) specific pore area (ap). Figure 3 schematically presents the scatter diagram of pores and dimensions of super active SAC-510 and Finix-112 catalysts.

**TABLE 6.** Results of the SAC-510 and Finix-112 powders

 based on BJH test

Variable	Unit	Finix-112	SAC-510
Pore Volume (V <sub>p</sub> )	Cm <sup>3</sup> /g	0.1231	0.1762
Pore Peak Radius (R <sub>p</sub> )	Nm	5.29	10.65
Specific Pore Area (A <sub>p</sub> )	m²/g	31.951	28.827



**Figure 3.** Scatter diagram of pores and dimensions of a) super active Finix-112 and b) SAC-510 catalysts. *Key*:  $V_p$  = Pore volume;  $R_p$  = Pore peak radius;  $a_p$  = Specific pore area

As seen in Table 6, the pore volume in catalyst SAC-510 was greater than that of Finix-112. This had an opposite effect on the specific surface and reduced this variable. Also as shown in Figure 3, the dVp/dRp ratios for SAC-510 indicate that the dispersion of the pores and sizes did not occur as uniformly as those found for Finix-112.

To assess the validity of the findings obtained through the BET analysis, we used BJH test (33). The advantage of BJH test is that it measures the volume and distribution of the pores while BET test provides a reliable measure of the areas associated with the solid material in the catalysts. Also, BJH test assists in obtaining approximate data regarding the absorption and release of isotherms, the pores' dimension, and their distribution within the catalysts.

**3. 5. Gel Permeation Chromatography** GPC-IR has been used to characterize the copolymer and the consequences are given in Figure 4 it is observed that the



**Figure 4.** GPC analysis diagram of product HDPE-100 with novel and commercial catalyst A) HDPE-100 obtained from commercial catalyst (Finix112): B) HDPE-100 obtained from novel catalyst (SAC-510)

bimodal molecular weight has been formatted. The copolymer received from the novel catalyst has a high branch degree in the high molecular weight fraction and lower branch degree in the low molecular weight fraction, that's favorable to enhance the resin mechanical properties.

The polymer properties are determined by the characteristics of the polymer including molecular weight, its distribution, and degree of branching. The breath of the molecular weight distribution, Mw/Mn, additionally affects the process ability of the polymer. The degree of short chain branching strongly influences a few variables together with crystallinity and density, which in flip determines the last properties of the material. The slurry polymerization processes give resins, which have great mechanical properties preserving wonderful process ability. It can be found out via bimodal high molecular weight HDPE. The low molecular weight component product in a single reactor offers suitable process ability, even as the high molecular weight component created with inside the different reactor offers exceptional mechanical strength.

**3. 6. Comparison of both SAC-510 and Finix-112 with Industrial Catalysts and Efficiency** Table 7 represents major important factors and performance about some currently used catalysts in chemical engineering science, as well as in industries, compared with the novel, super-active catalyst, SAC-510. All of the currently available catalysts have been used for the manufacturing of polyethylene pipes grade 100.

Hydrogen is the most broadly used chain-transfer agent for molecular weight control with Ziegler-Natta structures in industry. Hydrogen is the simplest commercially relevant chain-transfer agent in the lowpressure olefin polymerization process over the Ziegler-Natta catalysts. Valuable and important points aspects that are suggested from the data analysis, as shown in Table 7 in support of the super-active SAC-510 catalyst application toward the manufacturing of grade 100 polyethylene pipes are as follows: a) superior performance and durability; b) little consumption of triethylaluminum, 1-Butylene and hydrogen; c) better hydrogen response; and, d) ideal strength of the polyethylene pipes made of HDPE-100 product compared to other currently available industrial catalysts.

As can be seen in Table 8, the efficiency with the Sack catalyst has a considerable advantage over other catalysts in almost all parameters, such as reducing 1-butene consumption, reducing hydrogen consumption, reducing triethylaluminum consumption and increasing activity, and using this Catalyst is recommended in the production of polyethylene 100 product.

**3.7. Oxidation Induction Time** In Table 9, some characteristics of super catalyst product are listed with the products of other catalyst. The comparison of OIT in the product of the novel catalyst with the product of other catalyst shows an acceptable OIT and indicates the successful performance of the SAC-510 catalyst.

Oxidative induction time (OIT) is widely used for the determination of the thermal oxidative resistance of polyethylene materials The OIT testing only provides a relative measure of the level of antioxidants remaining in the pipe material but is a suitable analytical technique to monitor the degree of depletion of antioxidants from the pipe surface. Oxygen induction times (OIT) indicate the stabilities of the products (47). The concentration of effective antioxidant was assessed by determining the oxidation induction time (OIT) at 210 °C. The data presented on the deterioration of polyolefin pipes exposed to water containing chlorine dioxide have been mostly concerned with lifetime issues. Choosing a constant testing temperature which delivers OIT times of around 60 min for the unaged reference samples can be too high for the aged samples. On the other hand, a much lower temperature for OIT tests could result in high differences between the unaged and aged samples (48).

#### 4. LIMITATIONS OF THE STUDY

This study faced several challenges due to limited or lack of laboratory equipment and organic chemicals when it was being conducted as follows:

1. Lack of nuclear magnetic resonance facility to quantify the extent that butylene-1 was incorporated into the copolymer chains at 125°C.

2. Difficulty with separating 1- butylene from the solvent due to their close boiling points.

Catalyst	Unit	PE100/article	PE100/THS	PE100/BCE7	PE100/Finix-112	PE100-/SAC510
1-Butene Consumption	Kg/ton PE	18.51	21.21	15.6	16.8	15.5
H <sub>2</sub> Consumption	g/ton PE	1129.6	387	426	406	319
TEAL Consumption	Liter/ton PE	-	1.38	1.82	1.4	1.1
$Q_{RA}H_2\!/C_2H_4$	-	8	3.5	7.5	4.1	3.3
$Q_{RB}H_2\!/C_2H_4$	-	0	0.02	0.06-0.07	0.03	0.01
R <sub>B</sub> Pressure	Bar gauge	2.5	3.5-4	2.5-3	2.6	2.8
Activity	Kg PE/g Catalyst	8.82	20.6	20.75	27	28
R <sub>A</sub> Pressure	Bar gauge	-	-	-	-8.4	6.4

	<b>TABLE 7.</b> Results of the SAC-510	performance versus other industrial	catalysts at our site (32)
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TABLE 8. Results of the SAC-510 efficiency versus other industrial catalysts at our site (32)

Catalyst	Unit	SAC/article	SAC /THS	SAC /BCE7	SAC /Finix-112
1-Butene Consumption	%	19.42%	36.83%	0.6%	8.38%
H <sub>2</sub> Consumption	%	254.1%	21.31	33.54%	27.27%
TEAL Consumption	%	-	25.45%	67.27%	27.27%
$Q_{RA}H_2\!/C_2H_4$	%	142.4%	6%	127.3%	24.39%
$Q_{RB}H_2\!/C_2H_4$	%	0	100%	600%	200%
R <sub>B</sub> Pressure	%	-10.7%	33.9%	-1.78%	-7.14%
Activity	%	68.5%	26.42%	25.89%	3.57%
R <sub>A</sub> Pressure	%	-	-	-	31.25%

**TABLE 9.** Material properties of the reference samples (Mw: molecular weight, OIT: oxidation induction time at 210 °C, X: degree of crystallinity)

HDPE pipe	PE1(48)	PE <sub>2</sub> (48)	PE <sub>SAC-510</sub>	PE <sub>Finix-112</sub>
Molecular weight (M <sub>w</sub> )	115561	131344	241203	233372
OIT (min)	66	67	69	65
Crystallinity (%)	52	45	51.22	49.92

3. Inability to conduct mechanical strength and strain tests on the PE-100 pipe made of the novel catalyst. Ideal tests would include burst, hydro, and slow-crack-growth tests.

#### **5. RECOMMENDATIONS FOR FUTURE STUDIES**

We recommend the conduction of future researches with a focus on the following points:

1. Adjusting the use of hydrogen to improve control over the catalyst's molecular mass.

2. Testing other co-catalysts and investigating their effects on the morphology and activity of the resultant catalyst.

 Applying different organic solvents with higher boiling points to facilitate their removal from 1-butylene.
 Rheological and viscosity experiments on the polymer's long chains at zero shear rate.

#### 6. CONCLUSION

The prominent purpose of this research paper is the experimental production of a novel, cost-effective and efficient super-active catalyst (SAC-510) (patent pending), which is potentially ideal for manufacturing a wide range of high-density polyethylene pipes used in various industrial applications. The generation process of SAC-510 heterogeneous catalyst took place on a bed of magnesium ethoxide (as the co-catalyst), and halocarbon in the presence of titanium tetrachloride. The co-polymerization of ethylene and 1-butylene slurry was implemented in a Buchi's reactor under optimal conditions of temperature and barometric pressure.

Based on the SEM results, it was corroborated that the SAC-510 catalyst derives its active property from its spherical particles, in the presence of triethylaluminium in Buchi's reactor. Analysis of the obtained results from BET test demonstrated that the specific area for the pores in SAC-510 was 9% less than that of Finix-112. Also, the particle distribution of SAC-510 catalyst was about 60% greater than that of determined for Finix-112 catalyst, which demonstrates the superior efficiency of SAC-510.

Compared to other catalysts, the major advantages of SAC-510 are: a) the economical use of hydrogen and comonomers, b) better crystalizing capacity, and, c) low purge of valuable gases during the polymerization process. Further improvements on this subject await future research.

#### 7. ACKNOWLEDGEMENTS

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#### 8. SUPPLEMENTAL DATA AVAILABILITY

The detailed datasets generated and analyzed during the current study are available for review from the Corresponding Author upon request.

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چکيده

#### Persian Abstract

در این تحقیق، فرآیند سنتز یک کاتالیزور فوق فعال جدید به نام SAC-510 در مقیاس تجربی بررسی شده است. نویسندگان داده های تجزیه و تحلیل شده را با داده های به دست آمده از یک کاتالیزور پرکاربرد، Finix-112، و چندین جایگزین موجود دیگر مقایسه کردند. داده ها نشان داد که کاتالیزور SAC-510 بعالیت بهینه را از ذرات کروی خود به دست آورده است. تیتانیوم و سایر عناصر شیمیایی در SAC-510 با یکنواختی کمتری نسبت به نمونه های Finix-112 توزیع شده بودند، و اندازه متوسط ذرات در خود به دست آورده است. تیتانیوم و سایر عناصر شیمیایی در SAC-510 با یکنواختی کمتری نسبت به نمونه های Finix-112 توزیع شده بودند، و اندازه متوسط ذرات در آن ها کمی بزرگتر از اندازه موجود در 112-Finix بودند، و اندازه متوسط ذرات در آن ها کمی بزرگتر از اندازه موجود در 112-Finix بودند، و اندازه متوسط ذرات در آن ها کمی بزرگتر از اندازه موجود در 112-SAC و اندازه منافذ در 510-SAC به اندازه موارد موجود در کاتالیزور 112-112 به طور یکنواخت توزیع شده است. در نهایت، هر دو کاتالیزور 110-122 و اندازه منافذ در 510-SAC به اندازه موجود در کاتالیزور 110-112 به طور یکنواخت توزیع نشده است. در نهایت، هر دو کاتالیزور 110-122 و اندازه منافذ در 510-SAC به اندازه موجود در کاتالیزور 510-SAC و اندازه منافذ در 510-SAC به اندازه موجود در کاتالیزور 110-122 و یکنواخت توزیع نشده است. در نهایت، هر دو کاتالیزور 510-SAC و 112-Sinx به یک اندازه برای استفاده در لوله های پلی اتیلن با چگالی بالا (درجه ۲۰۰۰) سازگار بودند. در مقایسه با سایر کاتالیزورهای تجاری موجود، مزایای عمده 510-SAC استفاده اقتصادی از هودرون و مونوموها و پاکسازی کم گازهای از زمند آن در طول فرآیند پلیمریزاسیون است. سایر کاتالیزورهای تجاری موجود، مزایای عمده 510-SAC استفاده اقتصادی از هیدروژن و مونوموها و پاکسازی کم گارهای از در مول قران های موران و مونوموها و پاکسازی کم گارهای از زمند آن در طول فرآیند پلیمریزاسیون است. سایر کاتالیزور ماده میزان ۲۰.۲ درمد، اوزیش فعالیت به میزان ۲۰.۲ درمان زمان القای اکسبت به میزان ۲۰.۲ درمد، افزایش موجود. درمد، میزان ۲۰.۲ درمد، میزان ۲۰.۲ درمد، پاسخ دهی هیدروژن به میزان ۲۰.۲ درمد، میزان ۲۰.۲ درمد، میزان ۲۰.۲ درمد، میزان ۲۰.۲ درمد، میزان ۲۰.۲ درمد و نیز کاهش مصوف تری از ترد درمد، نور تور می میزان ۲۰.۲ درمد،



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# Smart City Surveillance: Edge Technology Face Recognition Robot Deep Learning Based

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## ABSTRACT

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Keywords: Convolutional Neural Network Deep Learning Edge Technology Face Recognition Smart City Security System In the contemporary context, the imperative to strengthen security and safety measures has become increasingly evident. Given the rapid pace of technological advancement, the development of intelligent and efficient surveillance solutions has garnered significant interest, particularly within the realm of smart city (SC). Surveillance systems have been transformed with the emergence of edge technology (ET), the Internet of Things (IoT), and deep learning (DL) to become key components of SC, notably the domain of face recognition (FR). This work introduces a smart surveillance car robot based on the ESP32-CAM micro-controller, coupled with a FR model that combines DL models and traditional algorithms. The Haar-Cascade (HC) algorithm is employed for face detection, while feature extraction relies on a proposed convolutional neural network (CNN) and predifined DL models, VGG and ResNet. While the classification is made by two distinct algorithms: Naive Bayes (NB) and K-nearest neighbors (KNN). Validation experiments demonstrate the superiority of a composite model comprising HC, VGG, and KNN, achieving accuracy rates of 92.00%, 94.00%, and 96.00% on the LFW, AR, and ORL databases, respectively. Additionally, the surveillance car robot exhibits real-time responsiveness, including email alert notifications, and boasts an exceptional recognition accuracy rate of 99.00% on a custom database. This ET surveillance solution offers advantages of energy efficiency, portability, remote accessibility, and economic affordability.

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#### **1. INTRODUCTION**

Technology is undergoing rapid and continuous transformation, exerting a profound impact on our daily lives. Our society is increasingly shaped by innovation, scientific progress, and the pervasive deployment of artificial intelligence (AI) in practical applications, including smart automobiles, robotic systems, and wearable devices like smartwatches and smartphones. In this context, ensuring security and safeguarding individuals have assumed unparalleled significance, given the extensive exchange and generation of data by this technological wave (1). The imperative of ensuring the safety and well-being of individuals has become an essential facet of modern life, particularly in the context of SCs. The overarching objective of SCs is to enhance the overall quality of life for their inhabitants, with a particular emphasis on security. This goal is achievable through the integration of advanced technologies, such as intelligent surveillance systems that incorporate cuttingedge components like smart video cameras, sensors, and data analytics techniques (2). The demand for surveillance systems is expanding, given their integral role in safeguarding individuals, preserving public safety, and facilitating efficient urban governance. As SCs continue to expand, the adoption of edge technology (ET) presents new opportunities and advantages. ET enables data processing and analysis in proximity to the data source, as opposed to relying solely on centralized systems. It is the convergence of ET and IoT that has reshaped the lives of millions, simplifying and fortifying virtually every aspect of their daily routines (3). ET, also referred to as edge computing, represents a paradigm where certain services are delivered in close proximity to, or directly on, the devices that initiate the requests (4, 5). This paradigm has contributed significantly to the transformative impact of technology on contemporary society. It provides a variety of advantages; we listed below some main points among them :

- Real-Time Response and Decision Making: ET enables immediate data analysis at the data source, enhancing public safety through rapid processing and response (6, 7).
- Scalability and Flexibility: Distributed architecture accommodates data growth, expands surveillance coverage, and supports real-time video analytics (8).
- Resilience and Reliability: ET's decentralization ensures uninterrupted surveillance, even during network disruptions or emergencies (6, 8).
- Cost Efficiency: ET reduces reliance on expensive cloud resources, optimizing resource use and lowering operational expenses (8).

Many and various industrial security solutions are based on these IoT, ET, and DL advanced technologies. Taking the example from literature (9), a DL-based blockchain-driven scheme for SC security. I this work, the blockchain aspect is employed in a distributed manner at the fog layer to secure the integrity, decentralization, and security of manufacturing data. DL is applied at the cloud layer to boost productivity, data automate processing, and increase the communication bandwidth of smart factory and smart manufacturing applications. They give a case study of vehicle production with the newest service scenarios for the proposed scheme and a comparison to previous research studies utilizing critical characteristics such as security and privacy tools. The solution comprises five layers: a device layer for data collection using physical IoT devices; an edge layer that contains industrial gateways for data communications; a cyber-layer blockchain-based to verify and validate the data; a data analytics layer for data processing and analysis using DL to extract knowledge; and an application layer that employs the knowledge and the results to realize selfmanagement, self-automation, scalable production, and rapid development in smart manufacturing.

Providing solutions that incorporate IoT and ET into the surveillance aspect is the need of the hour and what the researchers and scientists are striving to do, since it's characterized by various advantages but mainly high efficiency and a reasonable cost (2). For that, video surveillance is one of the most crucial and fundamental parts of ensuring security for SC. Providing new tools and methods that enable people to monitor, control, and increase the stability of the city with fewer human errors (2). This paradigm shift centers around real-time video streaming and data generation through intelligent ET and IoT devices, increasing image processing, collecting more vision data to analyze every day, and information extraction. Consequently, the visual component emerges as an essential element for smart biometric security applications (10). In particular, the FR systems, that play a significant role in enabling the identification of individuals based on their physiological, physical, and behavioral attributes (11). The human face, in this context, stands as a prominent element in biometric identification and verification. This method boasts several advantages, including user friendliness, contactless operation, remote applicability, and real-time decision-making (11, 12). The evolution of FR systems has witnessed substantial progress, transitioning from controlled environments to the processing of faces captured in uncontrolled settings and extending from traditional feature extraction techniques to the adoption of DL methods (8).

Various works and studies have been put out by researchers as for FR IoT and DL-based solutions. DLbased intelligent FR in an IoT-cloud environment is proposed by Masud et al. (12). This research suggests a tree-based DL for automatic FR in a cloud setting. As mentioned in the paper, the proposed deep model is

computationally less expensive without affecting accuracy. In the model, an input volume is split into numerous volumes, and a tree is produced for each volume. A tree is described by its branching factor and height. Each branch is represented by a residual function, which is made of a convolutional layer, a batch normalization, and a non-linear function. The proposed model is examined in standard databases. A comparison of performance is also done with state-of-the-art deep models for FR. The results of the experiments reveal accuracies of 98.65%, 99.19%, and 95.84% on the FEI, ORL, and LFW databases, respectively. Kumar et al. (13) suggested a framework using visual recognition for IoT-based SC surveillance. In this manuscript, a quick subspace decomposition over Chi Square transformation is proposed. This technique extracts the characteristics of visual data using a local binary pattern histogram (LBPH). The redundant features are removed by using rapid subspace decomposition over the Gaussiandistributed Local Binary Pattern (LBP) features. As mentioned in the paper, the redundancy removal is a major contribution to memory and time consumption for battery-powered surveillance systems, which makes the methodology suitable for all image recognition applications and deployment into IoT-based surveillance devices due to improved dimension reduction. The technique was implemented on the Raspberry Pi and validated over well-known databases. The least error rate is attained by the suggested technique with maximal feature reduction in minimum time, with 0.28%, 1.30%, 9.00%, and 2.5% rates over AR, O2FN, LFW, and Dyn Tex++ databases, respectively. Other FR-DL-based solution is presented by Charoqdouz and Hassanpour (14). The goal of this study is to estimate the feature vector of a full-face image when there are numerous angular facial images of the same individual. This method extracts the essential elements of a facial image using the non-negative matrix factorization (NMF) method. Then, the feature vectors are merged using a generative adversarial network (GAN) to estimate the feature vector associated with the frontal image. The experiments were made on the FERET dataset, which contains angular pose images with an angle of up to 40 degrees. As concluded by the research, the proposed strategy can greatly increase the accuracy of FR technology. Shahbakhsh and Hassanpour (15) provided a solution to increase the image resolution at the feature level and improve the accuracy of FR methods. The methodology is based on extracting the edges of the face image using LBP and unsharp masking techniques and then adding them to the input image as a preprocessing that can help the used GAN model extract the highfrequency information of the low-resolution data images. The GAN examines picture edges and reconstructs highfrequency information to preserve the facial structure. The experiments were made on the FERET database along with images from other datasets such as MUCT,

FEI, and Face94. The results demonstrated a considerable influence on the accuracy of FR in low-resolution photos compared to other state-of-the-art FR technologies.

DL, as a transformative facet of AI, has demonstrated remarkable performance not only in FR systems but also in various signal processing applications such as speech recognition, image recognition, and video recognition (16). Leveraging the inherent advantages of DL, IoT, and ET to construct intelligent FR security applications is not merely a contemporary pursuit but a pressing necessity. The fusion of these technologies offers the promise of delivering high-performance efficiency, aligning with the evolving needs of modern urban security (16).

The major contributions in the paper are: first, implementing a complex DL-FR system capable of making real-time decisions and predictions close to the IoT origin data source. Secondly, presenting a smart surveillance solution with a real-world ET robot application. Finally, we propose a SC surveillance solution that offers several advantages: low economic cost, less power consumption, portability, and remote utility.

The paper is divided into four sections. The first section described above highlights and discusses the research problem and presents the literature survey. The second section explains what the FR system is, what its essential phases are, and how it is functioning. The third section illustrates the suggested methodology based on approaches, techniques, and the materials used. The fourth section of the paper presents the experimental setup, results, and discussion. The last section concludes the paper.

#### 2. FACE RECOGNITION SYSTEM

Over the course of the previous three decades, FR has garnered significant attention as an efficient image analysis and pattern recognition tool (17, 18). This heightened interest is largely attributable to the advancements in relevant technologies, which have facilitated a diverse range of commercial applications across various domains. These domains encompass transportation, where FR is employed for person identification and passport verification; law enforcement, where it aids in tracking suspicious individuals and identifying criminals; smart homes, which utilize FR for intelligent access control; healthcare, with the implementation of patient tracking systems; and marketing, where FR facilitates smart payment and personalized advertising (14, 18, 19).

The functionality of the FR system entails the creation of additional subtasks in a pipeline that are essential for its proper execution; an illustration of these subtasks is presented in Figure 1.



Figure 1. Face recognition system

- Face detection: It's the initial phase in the system; it shows if the image contains a face(s) or not by determining human facial location and dimensions. A lot of methods and algorithms are proposed for this task; some of them, among others, are the HC method by Viola and Jones (20) to identify facial characteristics with Haar-like features. Dlib HOG (21), which employs support vector machines (SVM) in conjunction with histograms of oriented gradients. Dlib CNN (21) combines a maxi-mummargin object detector with a CNN to extract facial features. Another method is FaceNet (22), which is also based on CNN.
- Features Extraction: A key step that follows the detection phase consists of extracting the features, also called the signatures, which must be sufficient to represent a human face in the form of a vector, as we can call it, encoding the face. It is necessary to examine the uniqueness and individuality of the human profile (23). It should be mentioned that this process can be completed in the face detection step (17). Many different techniques can do this operation, such as deep neural nets like ResNet (23), FaceNet, and OpenFace (24). A novel technique was introduced by Firouzi et al. (25). An optimized hexagonal canny edge detection method. Images were first transformed to a hexagonal grid, followed by hexagonal image filtering using a Gaussian filter. Then, the magnitude and direction of gradients are estimated on the three axes x, y, and z. In the next stage, non-maximum suppression is applied to the amplitude and direction of gradients. Finally, threshold selection, double thresholding, untrue edge tracking, and edge removal are done successively to reach edges in the hexagonal domain.
- Classification: The encoders or the face vectors from the previous phase are classified into one of the classes offered during the training to make the

general decision of either a known or unknown person. So, at this final stage, we have the process of finding an image label with a level of confidence. It is based on using supervised learning algorithms, which are frequently employed to do this type of operation. At this point in the system outcome, we will be doing either identification by comparison to other faces in order to determine the person's identity or verification of the person, which entails matching one face to another for accomplishing tasks like guaranteeing access, for example.

#### **3. METHODOLOGY**

The suggested ET surveillance robot works via a webbased application applying a FR model based on DL. This section will describe all the aspects, including the main steps, methods, and tools used to build our system.

**3. 1. Face Recognition Study Proposal** The proposed FR models in this work were developed using multiple processes, as depicted in Figure 2. Each stage will be illustrated and discussed. Starting with data preparation and preprocessing, moving on to face detection, feature extraction, and classification. Each FR model will be a combination of several algorithms and DL models.

**3. 1. 1. Data Preprocessing** As we can see in Figure 2, the data section is divided into two parts: one for benchmarks and the other for a local dataset. Benchmarks are a common database used for FR problems; in this work, we chose three of them: the LFW, the ORL, and the AR database. Such databases are for validating our FR-proposed models. The first one is the LFW<sup>1</sup> database, which has 13233 images of 5749 people. The second is the AR<sup>2</sup> database, which contains over 4,000 images corresponding to 126 people's faces. The third is the ORL<sup>3</sup> database, which comprises 400 images, represented by 40 subjects that have 10 photos per subject.

Moving to the second part of data preparation, in order to acquire a successful, correct outcome, a substantial amount of training data is required, but on the other hand, it is difficult and challenging work to do in a real-time context. Therefore, we create our own database using the data augmentation approach. It is utilized to generate more and new samples by modifying the existing data images. This database is used for testing our proposed FR models to be deployed with surveillance car robot. Therefore, we combine three different human face pictures together; two of them were chosen randomly from the AR database, and the third was from the author

<sup>&</sup>lt;sup>1</sup> https://www.ece.ohio-state.edu/~aleix/ARdatabase.html

<sup>&</sup>lt;sup>2</sup> <u>https://cam-orl.co.uk/facedatabase.html</u>

<sup>&</sup>lt;sup>3</sup> http://vis-www.cs.umass.edu/lfw/

itself. Each image will be labeled with a class name, "Class\_0", Class\_1," and Class\_2," as shown in Figure 3.

The augmentation process is made by applying different operations as described and listed in Table 1. Using this strategy, we built a local database containing 2430 face images with 810 data images per class.

Reshaping all the images to 64 by 64 grayscale photos is another preprocessing step to guarantee that all the data have the same shape. Next, a normalization strategy will be employed to verify that all data are in the same range.



Figure 2. The proposed face recognition models



Figure 3. Local database classes labelling

<b>TABLE 1.</b> Data	augmentation	operations

Parameter	Interval or Value
Zoom	[-5, 5]
Shear	0.5
Height shift	0.3
Width shift	0.3
Rotation	[0, 15]

<sup>1</sup> https://github.com/fchollet/keras

**3. 1. 2. Face Detection** After preparing four distinct databases, a second step of face detection took place using HC. This algorithm uses a collection of predetermined features based on the foundation of Haarlike features, including edges, lines, and corners, as illustrated in Figure 4, to identify facial features like the eyes, nose, and mouth. It takes the frontal face as an input that will be exposed to a cascade application of the classifier. The image is divided into portions before the classifier is applied to each area. If a region is recognized as a face, the cascade continues to the next phase; otherwise, it is discarded, and the next region is processed. Figure 5 represents an example of this process.

**3.1.3. Features Extraction** CNNs have changed the domain of computer vision (CV) by imitating the human visual system's hierarchical processing. CNNs learn and extract internal representations or features straight from raw picture data, making them highly effective for tasks like FR, image categorization, object detection, and more. In this part, we will discuss the training process of our DL models. Three different DL models will be applied; two of them are predefined: the VGG (26) and the ResNet model. The third one is a proposed CNN built using the TensorFlow (27) and Keras<sup>1</sup> frameworks. Our suggested CNN is composed of 13 layers and has an architecture as explained in Table 2.

Following normalization, feature extraction and redundancy reduction take place in a pair of



Figure 4. The Haar features used in the HC algorithm



Figure 5. Haar features application over an image

Layer Type	Number of Layer
Two-Dimensional Convolutional Layer (Conv2D)	04 layers
Batch Normalization Layer	02 layers
Max Pooling Layer	02 layers
Dense Layer	03 layers

**TABLE 2.** Proposed CNN model architecture

convolutional layers coupled with pooling layers. Simple features come together efficiently over time. The features are then partially blended, with each resulting feature accounting for a portion of the configuration of the designated class. Finally, the fully connected layer receives these top attributes and delivers an estimation of the classification. To understand in more detail the process of feature extraction by the CNN, we have to illustrate each layer functionally. Figure 6 (28) shows a graphical representation of a CNN model where each layer is responsible for a specific operation.

Convolutional layers play the role of feature extractors. To generate feature maps, inputs are convolved with learned weights, and the results are then sent through a nonlinear activation function. Equation 1 specifies the output of the *kth* feature map, denoted by  $Y_k$ .

$$Y_{\mathbf{k}} = W_{\mathbf{k}} \odot M \tag{1}$$

where:

- $W_k$  is the convolution filter.
- The sign "©" refer to the 2D convolution operation.
- *M* refer to the input data image.

The batch normalization layer has the role of normalizing the input and tackling the vanishing gradient problems (16). It uses a normalization approach that takes place between the layers of the network instead of in the input data, in the form of mini-batches. By including additional layers, the learning process can be faster and more reliable. When a layer's input comes from a prior layer, the new layer standardizes and normalizes it.

For the pooling layer, as the name suggests, the operation of pooling or named subsampling also works as a bridge between several convolutional layers. The most popular pooling approaches in CNNs are maxpooling and average-pooling. It minimizes the spatial dimensions of the feature map, thereby lowering the computing process and aiding in translational invariance. In our study, we utilized the max pooling operation. It involves dividing the input feature map into regions called pooling windows and selecting the maximum value from each region. Equation 2 shows the process of this operation, where the output of this layer is denoted by  $Y_{\rm kij}$  representing the *kth* maximum element of a region from an image.



Convolutional Layer Convolutional Pooling layer Convolutional Pooling layer Layer Layer Layer Figure 6. CNN model graphical representation

$$Y_{kij} = maximum_{(p, q) \in R_{ij}} (M_{kpq})$$
(2)

where:

*M*<sub>kpq</sub> denotes *kth* element at location (*p*, *q*) from input data image *M* contained by the *maximum* of region *R*<sub>ij</sub>.

Figure 7 demonstrates even more this operation. A convolution layer's inputs are converted to the pooling layer's inputs. The greatest value in each 2x2 sub-area is mapped using a 4x4 mask.

After the feature extraction, the classification phase takes over, utilizing dense layers, which are completely connected layers employed to map the learned features to specific classes. These layers are critical for accurate classification and comprehending complicated relationships between features.

The training process for our DL models involved employing several parameters discussed as follows:

- Learning Rate: The learning rate controls how much the model's weights are changed during training. In our study, we fixed it to 0.001.
- Batch Size: Batch size defines the number of training samples utilized in each iteration of gradient descent, which in our case was 32.
- Number of Epochs: The number of epochs denotes the number of times the full training dataset is transmitted forward and backward through the network. We adjust it to 150.
- Optimizer: The optimizer governs the weight adjustments during training. Our DL models were trained using the RMSprop optimizer (29).

During the neural network training, a common challenge frequently addressed is the phenomenon known as overfitting. It occurs when the model learns to perform very well on the training data but fails to generalize to new, unknown input. As a solution to our work, three strategies are being applied, as given below:

• Regularization: One of the main methods employed is the integration of regularization techniques, such as L1 and L2 regularization. These methods contain penalty terms in the loss function, deterring the



Figure 7. Illustrative example of max pooling operation

model from allocating excessive value to certain features or parameters. This, in turn, promotes a more balanced model. In our case, we use the L2 method.

- Dropout: We add some dropout regularization that entails the random deactivation of a fraction of neurons during training, effectively introducing an element of unpredictability and preventing coadaptation among neurons. This enhances the network's ability to generalize by reducing reliance on specific neurons.
- Early Stopping: Monitor the validation accuracy during training and stop when it starts to drop. In order to apply it to our models, we use call-backs, an object that can perform actions at various stages of training. We fixed the monitoring operation for 30 consecutive epochs.

**3. 1. 4. Model Classifier** In this stage, we will use two supervised algorithms, the NB and the KNN, each at a time, to finish each FR model combination. The method is to classify the features encoded previously. The classification will be into one of the classes labeled with an amount of confidence, like a supervised classification strategy. It is about identifying and recognizing the face, and the result will be either a recognized person with a known label or an unknown person. After each training and classification phase, a model combination will be saved and exported for deployment purposes and to test our surveillance car robot. The best model of the sixmodel combination will be picked based on the accuracy results in the created database.

**3. 2. Edge Surveillance System Proposal** The suggested system in this study is predicated on the three parts detailed in the subsections below. The first one is the edge system, the second is the recognition system, and the third is the monitoring system, as indicated in Figure 8, where the functionality is as follows:

- Step 1: The edge surveillance robot captures the area with the camera module.
- Step 02: The recognition system captures the video transmitted by the robot, processes it, and extracts the images in real time.

- Step 03: If a face is detected, the FR model will take place and apply all the necessary steps to recognize it.
- Step 04: Presenting the outcomes on the live streaming web application, and also a notification email alert will be provided in case of unrecognized faces.

**3.2.1. Edge Surveillance System** Our proposed edge system is a surveillance car robot developed using several components, including:

- ESP32-CAM module.
- L298N Motor Driver
- Car robot that comes with 1 car chassis, 2 DC gear motors, 2 car tires, 1 universal wheel, 1 battery holder, and jumper wires.

Starting with the main module, the ESP32-CAM, which is a compact microcontroller and a low-cost ESP32-based development board featuring an inbuilt camera that works independently, powered by its own Wi-Fi and Bluetooth connectivity, among other specifications, as follows:

- Built in 520 KB of SRAM plus 4 MB of PSRAM.
- An SD card slot is supported.
- Built-in flash LED.
- The camera supports, which in our case, an OV5640 camera with a 5-megapixel image sensor.

The final result of the assembled car robot is represented in Figure 9.

After putting all the parts together and in order to make the system functioning, both for live streaming via the ESP32-CAM and for car robot control via the L298N motor drive, we have to program the ESP32-CAM board. Using the Arduino integrated development environment, we upload the main code written in C++ to synchronize the tasks between the components. The key functions are presented in Figure 10. Managing and using the robot will be done via a web application using a web browser.



Figure 8. The proposed face recognition surveillance system


Figure 9. Edge surveillance car robot

**3. 2. 2. Recognition System** We applied a preprocessing step to the live streaming video provided

through the ESP32-CAM module to extract the facial photos. Each video frame is turned into an image in order to identify the face inside it, after which features are extracted using DL models in order to classify them using the classification methods based on the confidence threshold.

**3.2.3. Monitoring System** The ability to drive the car and view the live streaming video using the same web application has been included as a final element in the proposed edge surveillance system, as shown in Figure 11. The buttons allow us to steer it in whatever direction we like while also managing the speed and lights. Our system has an email notification feature to alert users to unfamiliar faces as a security response.



Figure 10. Edge surveillance car robot main functions



Figure 11. Surveillance system web application

## 4. RESULTS AND DISCUSSION

The first part of our analysis will focus on the results of model validation toward benchmarks, while the second part will deal with the local data set that was developed to represent the results of the deployed model and the performance of the edge surveillance robot. The experiments made in this work, from training, testing, and validating the models, were using Google Colab [33], the free tier of the platform that delivers the needs with a system configuration as shown in Table 3.

TABLE 3. Google Colab	platform free tier configuration

Hardwar	Specifications
GPU	Nvidia Tesla K80
CPU	2x Intel Xeon @ 2.20GHz
RAM	13 GB
HARD DISK	78 GB

The model's performance evaluation was based on the accuracy metric as described in Equation 3.

$$Accuracy = \frac{TN + TP}{TN + TP + FN + FP}$$
(3)

where: TN (true negative) are the examples correctly classified as negative class; TP (true positive) are the examples correctly classified as positive class; FP (false positive) are the examples incorrectly classified as positive class; and FN (false negative) are the examples incorrectly classified as negative class.

**4. 1. Face Recognition Model Validation Results** As demonstrated in Figure 12, evaluating the models over the LFW, AR, and ORL databases provides different outcomes in terms of accuracy.

**4. 1. 1. LFW Database** The training set was 90% from this database, while the rest was for the testing set with 1330 samples using the train-test cross-validation. Each one of the model's combinations has its own accuracy. We can observe from Figure 12 that the best model with the highest accuracy over this database is HC + VGG + KNN, with a value of 92.00%.

**4. 1. 2. AR Database** As the first database, we apply cross-validation to get 10% of the data for testing with 400 samples. Analyzing the results of each combination represented in Figure 12 it is noticed that the HC + VGG + KNN model combination fit the best, with a 94.00% accuracy rate.

**4.1.3. ORL Database** The results demonstrate the accuracy of each combination in this database with a testing set of 40 samples with the same percentage of 10% from the whole database. Also, we notice that the HC + VGG + KNN model combination is the best, with 96.00% accuracy.

**4. 1. 4. Validation Results Summary** As a sum up of the model's validation process, we conclude that the HC + VGG + KNN combination provides the highest accuracy, as presented in Table 4. Observing that our models are affected directly by the number of classes, we notice that when the number of classes decreases, the accuracy of the models will increase.

**4.2. Surveillance System Results** In order to detail the suggested surveillance system results, we first represent the best model that was chosen for deployment into the system, where the combination was extracted after analyzing the model's accuracy results over the created database. Secondly, we represent the results of testing our surveillance car robot.

**4. 2. 1. Face Recognition Model Testing Results** The testing set had 10% of the database and 243 data



Figure 12. Model's performance over the benchmarks Model's performance over the benchmarks

<b>TABLE 4.</b> Comparison of the model's validation accuracy							
Databases	LFW	AR	ORL				
Models	with 5749 classes	with 126 classes	with 40 classes				
HC + VGG + NB	90.50%	92.00%	93.00%				
HC + VGG + KNN	92.00%	94.00%	96.00%				
HC + ResNet + NB	89.00%	91.00%	92.00%				
HC + ResNet + KNN	91.00%	92.50%	95.00%				
HC + CNN + NB	86.00%	88.00%	91.00%				
HC + CNN + KNN	88.00%	89.70%	92.00%				

samples. By observing the model performance, we found the best model, which consists of HC + VGG + KNN, has the highest accuracy rate of 99.00%. Starting with the confusion matrix represented in Table 5, the samples labeled "Class\_0" and "Class\_1", were all correctly classified, while the class labeled "Class\_2" had two miss-classified examples.

We can observe in Figure 13 the performance of the other models in terms of accuracy results. Noting that the HC + ResNet + KNN model also gives a high accuracy of 98.76% with a small deference to the chosen model.

**4. 2. 2. Face Recognition Deep Learning Model Testing Results** To do comparison analysis, we apply another training phase with the same parameters as mentioned earlier on the same local database using the CNN, VGG, and ResNet models, without the NB and

**TABLE 5.** Confusion matrix of the HC+VGG+ KNN model on local database

Predicted Class Actual Class	Class_0	Class_1	Class_2
Class_0	78	0	0
Class_1	0	83	0
Class_2	0	2	80

KNN classifiers. Aiming to observe the performance of these DL models since they can accomplish the classification task on their own. Figure 14 displays the test performance in terms of accuracy results. It indicates that this strategy of using the DL model for classification is superior to the approach of adding a traditional classification algorithm to the FR model. In terms of accuracy, the VGG outperforms the other models with a 99.15% rate, where we note 99.04% and 98.70% rates for the ResNet and the CNN, respectively.

To ascertain the robustness and effectiveness of each network architecture in terms of their performance, we added even more experiments based on accuracy and standard deviation for a series of experiments that were conducted repeatedly five times. The mean and standard deviation of the diagnostic accuracy are shown in Table 6. It can be concluded that the FR model based on HC and VGG outperforms all the other methods.

#### 4.2.3. Surveillance Robot System Testing Results

The surveillance car robot created throughout the research has been examined in a real-world setting to test its efficiency. The system's reaction was in real time, with an average of 0.30 seconds. The live video streaming provided by the robot will be analyzed and processed by the HC + VGG + KNN model, where it has successfully predictions over the captured face images. Figure 15 shows a system response inside a house environment to a known case where the face was successfully recognized.



Figure 13. Model's performance over local database



Figure 14. Deep learning model's performance over local database

TABLE 6. The mean and Standard deviation of accuracy results

		-
Metrics FR Models	Accuracy	Standard deviation
HC + VGG	99.22%	0.10
HC + ResNet	99.004%	0.12
HC + CNN	98.71%	0.17

To do more evaluations for the surveillance robot, we made some changes to the face positioning. The model was unable to recognize the features since it was not in frontal positioning, as represented in Figure 16a. We put our edge robot in another situation by changing the environment outside the house in cloudy weather, where it works as it should in terms of movements, video streaming, and image capturing, but the illumination affected the processing operations and the model was unable to recognize the face. The case scenario is illustrated in Figure 16b.



Figure 15. Edge system response for normal case scenario



**Figure 16.** (a) Edge robot response for non-frontal face scenario. (b) Edge robot response with bad lighting scenario

#### **5. CONCLUSION**

In this study, we developed a FR system based on DL and ET. We have successfully built an edge car robot that works with an implemented system that consists of various algorithms and a DL approach for SC surveillance. A notification feature is included in the system to alert the user about intruders or unidentified people nearby via email address. Our suggested solution has several advantages, including being a low-cost, affordable solution, less power-consuming, lightweight, supporting remote usage, and accomplishing the task of recognition in real time with high efficiency. This paper also demonstrates how edge devices with specific computational capabilities may now run complicated AI models while maintaining effectiveness and efficiency in terms of results. Further work and more aspects need to be covered, such as lightning changes since they affect the prediction results, face positioning, and face expressions, to give the model the best performance possible.

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#### Persian Abstract

چکیدہ

در زمینه معاصر ، ضرورت تقویت اقدامات امنیتی و ایمنی به طور فزاینده ای آشکار شده است. با توجه به سرعت سریع پیشرفت تکنولوژیکی ، توسعه راه حل های نظارت هوشمند و کارآمد علاقه قابل توجهی را به خود جلب کرده است ، به ویژه در قلمرو شهر هوشمند (SC). سیستم های نظارتی با ظهور فناوری edge (ET) ، اینترنت اشیاء هوشمند و کارآمد علاقه قابل توجهی را به خود جلب کرده است ، به ویژه در قلمرو شهر هوشمند (SC). سیستم های نظارتی با ظهور فناوری edge (ET) ، اینترنت اشیاء (IOT) و یادگیری عمیق (DL) به اجزای کلیدی SC تبدیل شده اند ، به ویژه حوزه تشخیص چهره (FR). این کار یک ربات ماشین نظارت هوشمند را بر اساس میکروکنترلر (IOT) و یادگیری عمیق (DL) به اجزای کلیدی SC تبدیل شده اند ، به ویژه حوزه تشخیص چهره (FR). این کار یک ربات ماشین نظارت هوشمند را بر اساس میکروکنترلر استان می مو کند ، همراه با یک مدل FR که مدل های DL و الگوریتم های سنتی را ترکیب می کند. الگوریتم Haar-Cascade (HC) برای تشخیص چهره (FN) استفاده می شود ، در حالی که استخراج ویژگی به یک شبکه عصبی کانولوشن پیشنهادی (CNN) و مدل های D پیش تعریف شده ، OGG و Totی است. در حالی که طبقه بندی توسط دو الگوریتم Autor (KNN) و مدل های D پیش تعریف شده ، OGP و ResNet میکی است. در حالی که طبقه بندی توسط دو الگوریتم متمایز ساخته شده است: ساده لوح Bayes (NB) و X-نزدیکترین همسایگان (KNN). آزمایشات اعتبارسنجی برتری یک مدل ترکیبی شامل OGG GE CK را شان می دهد و به ترتیب میزان دقت ۹۲.۰۰ × ۹۲.۰۰ × و ۹۲.۰۰ × را در پایگاه داده های HT را نشان می دهد و به ترتیب میزان دقت ۹۲.۰۰ × ۹۲.۰۰ × ۹۲.۰۰ × را در پایگاه داده های With است این نظارتی پاسخگویی در زمان واقعی را نشان می دهد ، از جمله اطلاعیه های هشدار ایمیل ، و دارای نرخ دقت تشخیص استفایی و ۱۳.۰۰ × را یک پایگاه بر این ، ربات ماشین نظارتی پاسخگویی در زمان واقعی را نشان می دهد ، از داه دول مورون به صرف بودن اقتصادی را ارائه می دهد.



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# Probabilistic Reactive Power Flow Optimization of Distribution System in Presence of Distributed Units Uncertainty Using Combination of Improved Taguchi Method and Dandelion Algorithm

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#### PAPER INFO

# ABSTRACT

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Keywords: Renewable Energy Improved Taguchi Method Orthogonal Arrays Optimal Reactive Power Distribution Dandelion Optimizer Uncertainty Nowadays, due to the growing population, rising global warming, environmental pollution, and the reduction of fuel sources, the use of Distributed Generation Sources (DGs) has grown, and because of their random nature, the conventional performance of power systems is being changed. Reactive power has a considerable role in power systems management and control indexes such as loss, stability, reliability, and security, among which the loss index usually can be easily minimized and controlled. Thus the modeling and optimizing of reactive power must be done accurately and correctly. This paper uses a novel metaheuristic algorithm which is called Dandelion, to solve the constrained non-linear optimal reactive power dispatch problem, and the Improved Taguchi method based on orthogonal arrays has been applied in order to the uncertainty of DG units modeling. The applied optimal reactive power dispatch algorithm is tested and validated using standard IEEE 30-bus test power systems. These results show that the Computational time of the applied algorithm in comparison with other used algorithms is the least value and reduces the reactive power from 22.244 to 2.366 Mvar; also, the losses of the power system significantly will be decreased with the tested and introduced algorithm. Genetic Algorithm(GA), Particle swarm optimization algorithm (PSO), and Prairie dog optimization algorithm (PDO) have been utilized to solve the problem.

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NOMECLAT	URE		
$V_{i}{}^{min}$ , $V_{i}{}^{max}$	The minimum and maximum voltage in the bus i, respectively.	$N_{exp}, n_g, N_C, N_T, N, N_B, N_L$	Number of experiments, generator, compensators, transformers,modules, buses, and lines, respectively.
$P_{\mathrm{i}}^{\mathrm{\ min}}$ , $P_{\mathrm{i}}^{\mathrm{\ max}}$	The minimum and maximum active power in the bus i, respectively.	GA, nb-1	Genetic algorithm, All basses except Slack bus, respectively.
$Q_{\mathrm{i}}^{\ min}$ , $Q_{\mathrm{i}}^{\ max}$	The minimum and maximum reactive power in the bus i, respectively.	OA, FF, WT, PV	Orthogonal Arrays, Full factor, Wind turbine, and Photovoltaics, respectively.
$s_{ij}^{\ max}$	Maximum apparent transmission power.	$V_{out}^{cut}$ , $V_{in}^{cut}$ , $V_{rated}^{cut}$ ,	The minimum, maximum, and nominal speed of the turbine.
$T_i^{max}, T_i^{min}$	The maximum, and minimum taps number of transformers, respectively.	Voc, I <sub>SC</sub>	Module open circuit/ short circuit voltage/ current, respectively.
$f_{j\psi},f^{*}{}_{\psi}$	The power and the nominal power passing through the $\psi$ transmission line and experiment j and , respectively.	$T_C$ , $T_a$ , $N_{OT}$	Photovoltaics, Ambiance, and Nominal operating temperatures, respectively.
$\sigma$ , $\mu,Y_j$	Standard deviation, Mean, and Test performance index, respectively.	Kv ,K <sub>I</sub>	Voltage and current temperature coefficient $\binom{A}{\sim C} \binom{V}{\sim C}$ , respectively.
$\overline{A}_j, P_d$	Average effects levels factor, Active demand power, respectively.	$V_{\text{MPP}}$ , $I_{\text{MPP}}$	Maximum power point voltage and current flow, respectively.
Level	The value of a random variable is based on an orthogonal array.	$\mathbf{V}_{\mathrm{i},\mathrm{j}}$	The voltage of bus i, and j respectively.
Delta	The main effect of random variables on performance indicators.	$\mathbf{G}_{\mathrm{i},\mathrm{j}}$ , $B_{ij}$	Line i – j conductance, and suspension respectively.
Rank, TM	Random variable class, and Taguchi method, respectively.	$Q_{ci,min}, Q_{ci,max}$	The minimum and maximum allowable reactive power generation, respectively.

## **1. INTRODUCTION**

Optimal reactive power dispatch (ORPD) is a major condition for the secure and economic operation of power systems, which will be reachable by suitable coordination of the system equipment used to manage the reactive power flow in order to reduce the active power losses.

The active power losses have been set as an objective in the ORPD problem. In order to achieve the desired objective, the generator bus voltages, and settings of passive devices such as transformers and shunt VAR compensators are adjusted to reduce the active power losses (1). The issue of reactive power control is vital in the distribution networks because if the consumption of reactive power in the distribution part has increased the power plants will not be able to produce more reactive power due to their technical limitations, so the losses will increase and thus the stability of distribution networks will change (2). Due to the reactive power consumption by the loads, the power factor of the distribution network will change, which will affect the network losses; according to technical concepts, the power factor must be near to one; of course, the unit power factor is an ideal state that will not be reachable (3). In distribution networks, capacitors have been used in order to loss reduction and also power factor correction, when the power factor has been decreased the reactive power will be injected into the network (4, 5). According to the above-mentioned statements explains, due to many consumed loads and transformers and generators, and other equipment, it is required to apply the optimal power flow (OPF) to control the reactive power because (6). Similar to OPF, the OPRD includes some continuous and discrete variables every one of them at least has one limitation, to solve the nonlinear problem, and

optimization of reactive power, using classic mathematics methods such as Gradient (7), Newton-Raphson (8), the interior point (9), linear programming (LP) (10), non-linear programming (11), and Quadratic programming (QP) (12). Enormous mathematical calculations and operations, getting stuck in local answers, are disadvantages of the mentioned classical methods (13). Using the metaheuristic method in order to solve the ORPD problem is strongly recommended because the mentioned disadvantages of the classical method will be eliminated. These algorithms are such as Whale Optimization Algorithm (WOA) (14), Particle Swarm Optimization (PSO) (15), Ant Lion Optimizer (ALO) (16), Improved Social Spider Optimization Algorithm (ISSO) (17), Improved Antlion Optimization Algorithm (IALO) (18), Genetic Algorithm (GA) (19), Ant Colony Optimizer (ACO) (20), Opposition-Based Gravitational Search Algorithm (OGSA) (21), Wind Driven Optimization Algorithm (WDO) (22), modified differential evolution algorithm (MDEA) (23).Specialized Genetic Algorithm (SGA) (24), evolutionary programming (19), comprehensive learning particle swarm optimization (25), fuzzy adaptive PSO (FAPSO) (26), seeker optimization algorithm (SOA) (27), cuckoo search algorithm (CA) (28), Hybrid Evolutionary Programming (HEP) (29), harmony search algorithm (30), Teaching Learning-Based Optimization (31), biogeography-based optimization (32), modified sine cosine algorithm (1), water cycle algorithm (33), hybrid Fuzzy- Jaya optimizer (34). With population and global warming increasing, the sources of fossil fuels are being decreased, so traditional power plants will have a problem in order to produce electrical power. These traditional power plants pollute the air and cause other environmental problems and have low efficiency (35). In recent years the use of DGs has increased. The produced electrical power of DGs depends on the intensity of sunlight, the angle of sunlight, wind speed, and the altitude of the turbine tower respectively in photovoltaic cells and wind turbines (36). These DG units, due to their random and probabilistic natures thus in OPF or OPRD should be used in probabilistic modeling methods. These DGs do not have the traditional power plants problems, even having high efficiency (37-39). According to the random nature of DG units, in order to convert uncertainties of their inputs the probabilistic modeling methods such as the Latin hypercube [26], point estimate method [27], scenario-based method [28], and Monte Carlo method, the Monte Carlo method is the basic method for any probabilistic assessment method [29], must be used. An optimization algorithm which is named improved social spider optimization algorithm (ISSO) has been used for optimizing the active and active power distribution, which is compared to the standard SSO, passes each process with two equations, using only one modified equation of the first and the second generations, creates the solution and has good and fast performance, less computation, less simulation time, and higher quality results in the ORPD problem than the standard SSO [31]. In order to solve the problem of ORPD, the water wave optimization algorithm (WWO) was used by Bhattacharya and Chattopadhyay [32]. The improved antlion optimization algorithm (IALO) has been used to solve OPRD and OPF for different constrained IEEE distribution networks, the good and accurate results in networks with bus voltage limitations and limitations of all capacitor banks prove that this algorithm is a powerful and accurate algorithm [33]. A new adaptive multiobjective optimization artificial safety algorithm has been used for OPRD, which is based on the Pareto coefficient, a method that is provided by Gafar et al. [34] for the classification of antibodies. Using the integration of three algorithms, particle swarm optimization (PSO), genetic algorithm (GA), and search for symbiotic organisms (SOS) (HGPSOS) to OPRD, which (SOS) has been based on the interactions between two various organisms which in the ecosystem - mutualism, hybridism, and parasitism are used. The HGPSOS algorithm has high computational speed and accuracy due to the presence of three precise and powerful algorithms, and it also has a high convergence rate, because it is combined with the GA, it shows that it is a stable and accurate algorithm [30]. Combining the heat transfer optimization algorithm (HTO) and the simulated coronary circulation system optimization algorithm (SCCS) was used by Zhang et al. [36] to reduce the losses and OPRD, each factor in the HTO algorithm is considered such as a cooling entity that is surrounded by other factors, like heat transfer, the thermodynamic law is used in the HTO algorithm. A candidate solution algorithm, which has been built and has been designed

from the mechanisms of the human body and capillaries, and is being used to optimize the OPRD and loss reduction, in this algorithm, the Coronary Development Factor (CDF) is responsible for the evaluation, and the initial population space has been selected freely, then in the whole population, the best solution is considered as the stem and the minimum value of the coronary will be expansion coefficient, then the crown production of the stem has been called the divergence phase, and the growth of other capillaries has been called the clip phase. According to the coronary artery growth factor (CDF), there will be superior capillary growth (BCL), With and without the L index (voltage stability). The (ORPD) problem, as a sub-problem of OPF, has significant effects on providing reliability and economical performance [37]. A new optimization algorithm which has been named Turbulent Flow Water Based Optimization Algorithm (CTFWO) is used to solve the OPRD which is a complex mixed integer nonlinear optimization problem that includes discrete and continuous control variables (40). The Benchmark table was utilized by Kumar et al. (41), which could be an enormous table with awfully expansive numbers that need much time and calculations to run for OPRD while the improved TM, employs OAs that have lower numbers and need lower time and calculations to run for the ORPD problem. The TM is a statistical and quality-control-based strategy (42) that is utilized to show the vulnerabilities of DGs, and OPF calculations using the relationship and correlation concepts of RVs while the improved TM is being utilized in the MINITAB and MATLAB computer software that the relationship and correlation concepts of RVs run automatically in the computer programs. The improved TM is accurate and has lower computational levels than TM, the time, and speed of converge are quick. to assess the capability of the Dandelion calculations and improved TM to solve the ORPD, the simulation results of the Dandelion algorithm calculation are compared with varied algorithms, including PSO, GA, HGPSOS, HTO, PDO, ISSO, WWO, and IALO. The calculations and the results of PSO, PDO, DO, and GA are compared and discussed in thr presentation of results. Furthermore, the results of the improved TM are compared with the results of the assessed execution of different POPF methods in Tables 3 and 4. The results show that the Dandelion algorithm calculation has the finest response, and is excellent in comparison to other algorithms in terms of arrangement precision, joining rate, and solidness. The improved TM is accurate in comparison to the TM and employs data amid the optimization process in other words, utilizing the POPF results amid optimization and the correlation of RVs, the discharge variable is required for more examination and optimization with more precision afterward in arrange to assess the productivity of the displayed strategy.

The notable contributions of this study can be categorized as follows:

1) Solving ORPD problem considering uncertainties of DG units and Time-varying load.

2) Applying the Improved Taguchi method for modeling load, solar irradiance, and wind speed uncertainties.

3) Using a new optimizing algorithm for solving the ORPD problem with and without DGs presence.

4) Comparing the performance of the Dandelion algorithm with the GA, PSO, and PDO for solving the ORPD problem.

#### 2. FORMULATION OF THE PROBLEM

In this section, the objective function of the OPRD problem is equal to loss minimization of the distribution network using reactive power optimization which has been expressed as Equation (1).

$$P_{Loss} = \sum_{l=1}^{nl} G_{ij} (V_i^2 + V_j^2 - 2V_i V_j \cos \delta_{ij})$$
(1)

The minimization of the objective function is being limited by various constraints, such as Equations 2 and 3 which show equal limits in the network, indexes G, and D have been applied to represent generation, and demand respectively. Equations 4 and 5 express unequal constraints which include the voltage constraints of generators, tap transformers, and the reactive power of compensating equipment. The taps of the transformers are also limited in their minimum and maximum range according to Equtaion 6. The constraints of parallel compensators are also according to Equtaion 7. In addition to these restrictions, according to Equtaion 8. The three main parameters in this function are:  $V_{rated}$ ,  $V_{in}$ , and  $V_{out}$ . When the wind speed reaches  $V_{in}$ , the WTs start generating power; when the wind speed reaches  $V_{rated}$ , the output power reaches the nominal  $P_{rated}$ . If the wind speed exceeds Vout, power generation will be stopped [25]. From a probabilistic aspect, the outputs can no longer be called definitive. In other words, all the outputs of the problem will be presented as mathematical expected values. This means that in this case, the outputs of losses and voltages are the mathematical expected values of voltages and losses.

$$PG_i - PD_i = V_i \sum_{j=1}^{nb} V_j \left( G_{ij} \cos \delta_{ij} + B_{ij} \sin \delta_{ij} \right)$$
(2)

$$QG_i - QD_i = -V_i \sum_{j=1}^{nb} V_j \left( G_{ij} \sin \delta_{ij} - B_{ij} \cos \delta_{ij} \right)$$
(3)

$$QG_i^{\min} \le QG_i \le QG_i^{\max} \tag{4}$$

$$VG_i^{\min} \le VG_i \le VG_i^{\max} \tag{5}$$

$$T_i^{\min} \le T_i \le T_i^{\max} \tag{6}$$

$$QC_i^{\min} \le QC_i \le QC_i^{\max} \tag{7}$$

$$V_i^{\min} \le V_i \le V_i^{\max} \tag{8}$$

**2. 1. Uncertainties Modelling** In probabilistic planning, it is important to state an appropriate statistical model for RnVr s, and it is being used in some models of uncertainty sources such as PV, WT, and electrical vehicle (EV) which the EV can charge at parking in smart distribution networks and can control the network indexes such as losses, voltage drop (43, 44).

**2.2. Load Modelling** Using normal distribution, the density function of the corresponding probability distribution has been expressed in Equtation 9:

$$f(P_d) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(P_d - \mu)^2}{2\sigma^2}\right)$$
(9)

**2. 3. Wind Turbine Modeling** The modeling of wind has consisted includes two steps, as follows:

I) **Wind speed modeling:** Due to the wind speed having random behavior, the wind speed must be modelled using a proper statistical distribution, and usually, to do so the continuous Weibull probability distribution is utilized according to Equtation 10.

$$f(v) = \frac{h}{c} \left(\frac{v}{c}\right)^{h-1} \exp\left(-\left(\frac{v}{c}\right)^{h}\right)$$
(10)

in the above-mentioned equation, v, c, and h represent the wind speed, the shape factor, and the scale factor respectively.

II) **Turbine output power modeling:** depends on the wind speed and other parameters of the wind turbine, which has been explained in Equtation 11.

$$p = \begin{cases} 0 & V_{out}^{cut} \le V \text{ or } V \le V_{in}^{cut} \\ K_1 V + K_2 & 0 \le V \le V_{in}^{cut} \\ P_{rated} & V_{rated} \le V \le V_{out}^{cut} \end{cases}$$
(11)

 $K_1 = \frac{V_{rated}}{V_{rated} - V_{in}} K_{2} = -K_1 V_{in} K_1$  V is the wind speed.

The details of power generation using wind turbines are shown in Figure 1.

**2. 4. Photovoltaics Modelling** Due to the sunlight radiation having random behavior, the radiation should be modeled using an appropriate statistical distribution, and usually, to do so the continuous Beta probability distribution is used according to Equtaion 12-a, using Equtaions 12-16 the active power can be calculated.

$$F(G) = \frac{1}{G\sigma\sqrt{2\pi}} exp\left[-\frac{\ln(G-\mu)^2}{2\sigma^2}\right]$$
(12-a)

$$P_{pv}(s) = N * FF * V(s) * I(s)$$
(12)



Figure 1. Wind turbine production capacity

$$V(s) = V_{oc} - K_V * T_C$$
(13)

$$I(s) = s * (I_{SC} + K_I * (T_C - 25))$$
(14)

$$T_c = T_a + s * \left(\frac{N_{OT} - 20}{0.8}\right) \tag{15}$$

$$FF = \frac{V_{MPP} * I_{MPP}}{V_{OC} * I_{OC}}$$
(16)

## **3. ORTHOGONAL ARRAYS**

An OA is a fractional factorial matrix whose rows represent factor levels in each run and its columns represent a specific factor whose levels change in each experiment. All traditional factorial designs and fraction arrays are orthogonal. In the past, OA was known as magic squares. Perhaps the effect of OA in experiments has led to such naming. Because a fraction of the experiments is chosen in it, each combination is repeated in equal numbers, the reason they are named orthogonal is that all the columns are examined independently. The OAs are denoted by the letter L, which comes from the Latin word because the use of OA in experimental designs is related to Latin square designs. An OA is basically a table whose rows are used for experiments and whose columns are used for an RnVr (Table 1). Each of the numbers in the table describes the modes of a RnVr. OAs are sorted with the symbol  $OA_{N_{exp}}$   $(N_L)^{N}$ .

For example, Table 2 is used for a problem with seven random variables and eight experiments; each random variable has two levels. Generally, must be done 128 processes, but by using the OA just eight experiments are needed. So, the calculation steps will be decreased to 6.25% of the total steps; this shows the ability and Advantage of OA (45, 46).

#### 4. IMPROVED TAGUCHI METHOD

The improved Taguchi method is to increase the accuracy of the Taguchi method and the flowchart of this method

**TABLE 1.** Orthogonal array  $OA_{N_{err}}$   $(N_L)^N$ 

E	Levels				
Experiment number	RnVr1	RnVr <sub>2</sub>		RnVr <sub>N</sub>	
1	L <sub>11</sub>	L <sub>12</sub>		$L_{1N}$	
2	L <sub>21</sub>	L <sub>22</sub>		$L_{2N}$	
N <sub>exp</sub>	$LN_{exp^{1}}$	$LN_{exp^2}$		$LN_{expN}$	

TABLE 2. Orthogonal array OA <sub>8</sub> 2	2'	
---	----	--

Experiment	Level of each variable						
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	2	2
6	2	1	2	2	1	1	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

is discussed as illustrated in this section. In this method, steps 1 to 5 of the Taguchi method, and the Improved Taguchi method are exactly repeated, but in the following, other steps are also performed. By comparing sets 1 and 2, probably some of the same variables will have the same levels. These variables are called certain variables and other variables are called uncertain variables. The reason for this naming is that are being obtained the same levels for these variables from two different paths, one of the experiments and the other of averaging the values obtained from the experiments. Certain variables are excluded from the optimization process. In the next section, the sixth step, the placement process is explained.

4. 1. Placement of Uncertain Variables in the **Experiment with the Best Value** The experiment that has the best result among the experiments performed is one of the possible experiments to examine all combinations of different variables. Therefore, there may be another combination of variables that has a better outcome compared to the current best available test. One of these more suitable combinations may be the combination corresponding to the best experiment, while its uncertain variables are placed according to set 2. Because the averaging of the obtained results was the basis for choosing set 2, the statistical nature of this process increases the probability of choosing the optimal values for the variables. The certain variables determined by the task are removed from the process and only the uncertain variables are re-examined. In order to prevent the interaction of variables, the process of placing

uncertain variables from the second set in the best experiment is done individually. If the inserted variable causes a better result than the previous variable, we call this variable definite and fix it in the best test. Other uncertain variables will be placed in the same way.

**4. 2. Choosing the Orthogonal Array for the Remaining Uncertain Variables** In this stage, uncertain variables are optimized by using another Taguchi table that is selected for them. If the number of remaining variables is small, we test all possible combinations. The optimization process continues until the optimization completion condition is met.

4. 3. The Differences between the TM and the Improved TM In the TM, finally, the levels of the RVs in sets 1 and 2 are placed in the best experiment, and each of the two sets that bring a better result is considered as the set containing the optimal values. In the improved TM, the RVs are divided into two groups of certain and uncertain variables. Certain variables are determined and removed from the optimization process. While the uncertain variables are checked more carefully, this is the difference between the improved TM and the TM. Since the presented method uses the TM, there is no need to prove the convergence towards the optimal point. To prevent the interaction of variables, the improved TM suggests the placement of individual variables. In this paper, the aim is to show the effect of the high precision of the simulation results of the Improved TM utilizing the Dandelion algorithm.

#### **5.DANDELION ALGORITHM**

A new swarm intelligence bioinspired optimization algorithm that has low computational time and high convergence speed has been called the Dandelion algorithm (DA) which has been introduced recently (47). Dandelion algorithm flowchart is shown in Figure 2. It includes three stages,

1. Growth stage: In this stage, the seeds spiral down from a high height due to eddies, or they are driven locally due to different climatic conditions.

2. Descending stage: In this stage, the flying seeds decrease their height by continuously adjusting their direction.

3. Landing or sitting stage: In this stage, the seeds descend to grow and grow in places they have chosen randomly. Using Brownian motions and Levy's random walk, the movement path of grains is determined in the stages of decline and settlement, respectively.

#### **6.0PRD USING IMPROVED TM**

In Improved TM every uncertainty is named as a random variable (RnVr). In general, the relationship between



Figure 2. Dandelion algorithm flowchart

input and output RnVr s in a distribution network is expressed according to Equation 18:

$$Y_{\rm in} = f \left( X_{\rm out} \right) \tag{18}$$

The f is a nonlinear relation that establishes the relationship between Xout and Yin. In OPRD, the factors are the same as RnVr s. In OPRD, the number of factors is expressed in m and the number of levels in n, and then the next mn test must be performed. In this paper, an OPRD of a distribution system that includes PV and WT DGs is investigated and analyzed using Improved TM based on OA.

In order to solve the OPRD problem:

(i) The structure and information of the power system equipment are important and practical.

(ii) The input RnVrs are shown by the vector  $Y_{in}$  according to Equation 18.

(iii) "Level" means the value below the curve is a function of the probability density of incoming RnVr s.

(iv) Every experiment refers to a load flow, if there are several RnVr s, thus the number of load flows will be increased, thus the final answer will be obtained after a long computational time and several mathematics operations. As the above- mentioned advantage of OA, thus should be used. The first step in deploying Improved TM is to determine the levels of each RnVr. Selecting two levels and three levels for each factor requires the least and most time and calculations, respectively. In Improved TM, levels 1 and 2 are being selected, respectively  $\mu$  -  $\sigma$  and  $\mu$  +  $\sigma$ . In the TM, the final optimal answer is being reached using an optimal experiment based on the optimal levels of RnVr s instead of all experiments based on OAs. To use this optimal experiment, one must first express an index according to Equation 19.

$$Y_{j} = \sum_{\psi}^{NL} \left| f_{j\psi} - f^{*}_{\psi} \right| \quad j = 1.2.3...$$
(19)

The second step is to determine the average effect of the factors based on Equations 19 to 25.

The third step is to define the main effect of each factor on  $Y_j$ . These main effects of the factors are being calculated according to Equations 26 to 29:

$$\bar{A}_1 = (Y_1 - Y_2)/2 \tag{20}$$

$$\bar{A}_2 = (Y_3 - Y_4)/2 \tag{21}$$

$$\bar{B}_1 = (Y_1 - Y_3)/2 \tag{22}$$

$$\bar{B}_2 = (Y_2 - Y_4)/2 \tag{23}$$

$$\bar{C}_1 = (Y_1 - Y_4)/2 \tag{24}$$

$$\bar{C}_2 = (Y_2 - Y_3)/2 \tag{25}$$

$$\Delta A = (\bar{A}_2 - \bar{A}_1) \tag{26}$$

$$\Delta B = (\bar{B}_2 - \bar{B}_1) \tag{27}$$

$$\Delta C = (\bar{C}_2 - \bar{C}_1) \tag{28}$$

If the major effect is positive in RnVr or the same factor, the second level is considered otherwise.

It is now shown how to apply the OAs to the OPRD by performing the following main steps:

- a) Determining the input RnVr s.
- b) Determine the number and values of the levels of variables.
- c) Determine the OA.
- d) Execute OPRD.
- e) Analysis of results.

$$\mu_{j} = \frac{1}{Nexp} \sum_{i=1}^{Nexp} x_{ji} \quad , \sigma_{j} = \left[ \frac{(\sum_{i=1}^{Nexp} x_{ji} - \mu_{i})^{2}}{Nexp} \right]$$
(29)

 $x_{ii}$  is the value of the j<sup>th</sup> output RV for the i<sup>th</sup> experiment.

#### 7. SIMULATION RESULTS

In this study, the 30-bus IEEE standard system has been used in order to solve ORPD. This system includes 6 generators and 80 transmission lines, of which 17 lines have a tap changer. Also, three reactive power compensating equipment, which are installed in buses 15, 25, and 53, have been used for compensating. The initial active, and reactive power loss of the network without the presence of DGs are 22.244 Mvar and 17.59 MW respectively. The performance range of the variables is given in Table 3 and other network information has been obtained from (48). The Improved TM is tested in MATLAB and MINITAB software. In this study, there are two wind farms in bus 38, 39 and a PV cell in bus 16,

**TABLE 3.** Values of  $\mu$  and  $\sigma$  using other methods

Entire losses	ТМ	Scenario	LHS	2PEM
μ [MW]	30.5	40.8	52.42	36.3
σ	11.15	26.1	36.22	12.2

which has a nominal capacity of 100 MW. To simulate this wind farm and PV cell, data has been received from the North Dekta site and the Watford area (49). Figure 3 shows IEEE 30-bus test system. The results are illustrated in Figures 4 and 5 show the converged plot of GA, PDO, DO, and PSO algorithms. Any of the optimizations have been run in 100 Iteration and more information about any optimization algorithms is explained below:

**7. 1. Genetic Algorithm** This optimization has been run in 26 populations and 100 iterations and in 44.076 (s). The number of the control variables is 13 and the percent of crossover is 0.1 and the best value for OPRD with GA is 3.891 MVar.



Figure 3. IEEE 30-bus Test system



Figure 4. Reactive power optimization with algorithms



Figure 5. GA, DO, PDO, PSO Buses Voltage

**7. 2. Particle Swarm Optimization Algorithm** This optimization has been run in 26 populations and 100 iterations and in 21.940 (s). The number of the control variable is 13 and the inertia weight is 1 and inertia weight damping ratio is 0.99 and personal learning coefficient is 1.5 and global learning coefficient is 2 and the best value for OPRD with PSO is 2.038 Mvar.

**7. 3. Prairie Dog Optimization Algorithm** This optimization has been run in 26 populations and 100 iterations and in 82.830 (s). The number of the control variables is 13 and the best value for OPRD with PDO is 3.584 MVar.

7.4. Dandelion Algorithm This optimization has been run in 26 populations and 100 iterations and in 19.996 (s), and the number of the control variables is 13 and the best value for OPRD with DA is 2.366 MVar according to Figure 6. Table 4 shows in terms of optimal value the PSO has a minimum value for OPRD and in terms of time the DA has a minimum value for OPRD so an algorithm that gives the best value in terms of time and optimal value for OPRD must be used and must be selected, according to Table 4 the PSO has a minimum value and maximum time even that time is equal to quadruple of DA time, but with pay attention to Table 4, the DA has closet value to PSO just with 0.3 MVar difference also has minimum time for solving of OPRD so the DA should be in OPRD problems. Before the use of the algorithms, the reactive power of 30 bus IEEE standard network was solved in 0.083(s) was equal to 22.244, and with paying attention to Table 4, it is concluded that the DA has closet time and much difference with the reactive power before using the optimization algorithms. using DA 20.2 MVar reductions will be had in reactive power which will be effective in terms of power losses and power transfer for power systems. Table 3 shows other probabilistic assessment methods such as point estimation, Taguchi, Scenariobased, and Latin hypercube sampling and their results.

Flowchart of improved Taguchi method is illustraed in Figure 6.

TABLE	4.	Results	of	OPRD	before	and	after	using	the
algorithm	ıs								

Algorithms	GA	PDO	DO	PSO	OPF
Time (s)	28.7	99.002	22.119	19.493	0.083
Reactive (MVar)	3.9611	3.0206	2.0917	2.2106	22.244
Buses Voltages (v)	0.8429	0.8298	0.8301	2.0410	
Time(sec)	19.207	82.022	18.827	21.940	



Figure 6. Flowchart of improved Taguchi method

#### 8. CONCLUSIONS

The loss is an important index for power systems that can be controlled by reactive power, thus it is necessary to optimize the reactive power by increasing the DGs in

power systems. In this paper, the dandelion optimization algorithm, and the improved Taguchi method which is based on orthogonal arrays have been utilized to solve complicated optimal reactive power dispatch problems and the modulation uncertainties of DG units, respectively. The use of portable systems such as wind turbines and photovoltaics as the most used technologies been considered. Moreover, the load and has uncertainties of wind turbines and photovoltaics have been investigated. The results show that the Dandelion algorithm has solved the OPRD in minimum time and has decreased the reactive power by about 20.2 Mvar which will be very good for the power system in terms of power losses and other aspects. Thus it is concluded that the Dandelion optimization algorithm and the Improved Taguchi method are effective, and accurate in solving the probabilistic ORPD problem compared with algorithms (GA, PDO, and PSO) applied for the ORPD problem.

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امروزه با توجه به رشد روزافزون جمعیت، افزایش گرمایش زمین، آلودگی محیط زیست و کاهش منابع سوخت فسیلی، استفاده از DG ها رشد کرده و به دلیل ماهیت تصادفی آن ها، عملکرد متعارف سیستم های قدرت در حال تغییر است. توان راکتیو نقش قابل توجّهی در شاخص های مدیریت و کنترل سیستم های قدرت مانند تلفات، پایداری، قابلیت اطمینان و امنیت دارد که در این میان معمولاً شاخص تلفات را می توان به راحتی به حداقل رساند و کنترل کرد. بنابراین مدل سازی و بهینه سازی توان راکتیو باید به طور دقیق و صحیح انجام شود. در این میان معرفر شاخص تلفات را می توان به راحتی به حداقل رساند و کنترل کرد. بنابراین مدل سازی و بهینه سازی توان راکتیو باید به طور دقیق و صحیح انجام شود. در این مقاله از یک الگوریتم فرابتکاری جدید به نام قاصدک برای حل مسئله توزیع توان راکتیو بهینه غیرخطی محدود شده استفاده می شود و همچنین از روش تاگوچی بهبود یافته مبتنی بر آرایه های متعامد برای مدل سازی عدم قطعیت واحدهای DG استفاده شده است. الگوریتم توان راکتیو بهینه عبرخطی محدود شده استفاده می شود و استفاده از روش تاگوچی بهبود یافته مبتنی بر آرایه های متعامد برای مدل سازی عدم قطعیت واحدهای DG استفاده شده است. الگوریتم توزیع توان راکتیو بهینه غیرخطی محدود شده استفاده می شود و استفاده می شود و استفاده شده است. الگوریتم توزیع توان راکتیو بهینه اعمال شده با استفاده از روش تاگوچی بهبود یافته مبتنی بر آرایه های متعامد برای مدل سازی عدم قطعیت واحدهای DG استفاده شده است. الگوریتم اعمال شده با سایر استفاده از روش تاگوچی بهبود یافته مبتنی بر آرایه های متعامد برای مدل سازی عدم قطعیت واحدهای DG استفاده شده است. الگوریتم اعمال شده با این استفاده از روش تاگوچی بهبود یان راکتیو بهینه اعمال شده با سایر الکوریتم های مورد استفاده کمترین مقدار را دارد و توان راکتیو را ز کاری و تایند می شود. این نتایج نشان می دهد. همچنین تلفات سیستم قدرت با الگوریتم تست شده و معرفی شده به میزان قابل توجهی کاهش می یابد. الگوریتم ژنتیک (GA) ، الگوریتم بهینه سازی مورد این معینی تلفات سیستم هی ی مشکل استفاده شده شده شده می یابد. الگوریتم ژنتیک (GA) ، الگوریتم بهینه می و در ای و اگوریتم بهینه می و یا یا در ای و ای ای در و ای ای در و و ای بر رای و ای ای در و ای و ای و در و ای در و و ای ای و راز و رازی و و و و در و و و و و و و و



# چکیدہ



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# Effect of Al<sub>59</sub>Cu<sub>25.5</sub>Fe<sub>12.5</sub>B<sub>3</sub> Quasi-crystals on Microstructure and Flexural Strength of Aluminum Matrix Composites Prepared by Spark Plasma Sintering Method

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#### PAPER INFO

### ABSTRACT

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Keywords: Quasi-crystals Al Matrix Spark Plasma Sintering Mechanical Properties In this study, Al-based composites reinforced with  $Al_{59}Cu_{25.5}Fe_{12.5}B_3$  quasicrystal (QC) were prepared by spark plasma sintering (SPS) method. Microstructural and mechanical properties were examined. It is observed that with addition of quasi-crystalline reinforcement the intensity of the quasi-crystalline peak has increased. Also, it is observed that by performing spark plasma sintering, the quasi-crystalline particles maintain their stability. Due to low temperature of the process and the short time of spark plasma sintering, the occurrence of destructive phases within the quasi-crystal has been prevented. based on field emission scanning electron microscopy (FESEM) images, the distribution of quasi-crystalline particles at the sample level has increased. In addition, the mechanical properties are improved by increasing the quasi-crystalline particles. Therefore, the sample with 15 vol.% of quasi-crystal has better results than other samples in improving microstructural and mechanical properties and it can be considered as an optimal sample with suitable practical properties.

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## **1. INTRODUCTION**

After classifying solids into two categories of crystalline materials and amorphous materials, guasi-crystals were introduced as the third type of solids by Avar et al. [1] and Shechtman et al.(1, 2). The quasi-crystals are among the new materials that have a non-periodic long-range order (3, 4). There is a repetitive periodicity in the arrangement of atoms with a forbidden rotational symmetry for the crystals in the quasi-crystalline material. Symmetries in quasi-crystals have been observed. Icosahedral, octagonal, decagonal and dodecagonal structural are among the most important quasi-crystals (2, 4, 5). There are several methods for the synthesis of the quasi-crystalline materials, these methods are: melt spinning, casting, mechanical alloying, gas atomization, physical vapour deposition (PVD), sol-gel, electrodeposition, gas evaporation, plasma spray and laser- or electron-beam superficial fusion and electron irradiation (4). One of the most widely used methods for the synthesis of quasi-crystals is mechanical alloying (MA) (3, 6). This method is a powder method that produces homogeneous materials from a mixture of pure powders. Mechanical alloying method has been used over the years as an acceptable fabrication method for the development of a variety of advanced materials such as nanomaterials, quasi-crystals, amorphous materials and nanocomposites (7, 8). The most important mechanisms of this method are repeated welding, fracturing, and re-welding of particles (9). Metal matrix composites (MMCs) consist of two main components including the matrix phase and reinforcement phase. The purpose of placing a highperformance secondary phase in these materials is to create a combination of aspects that would not be possible by the components alone. The reinforcement phase is continuous or discontinuous in the matrix. The reinforcement phases are continuous or discontinuous in the matrix, which may make up about 10 to 60 volume percentage of composite. The purpose of creating reinforcement phase in these materials is to achieve the desired properties that these properties will not be possible by the components alone (10). One of the most important and widely used metal matrix composites are aluminum matrix composites (AMCs) (10). Aluminum matrix composites are advanced engineering materials that have superior properties compared to conventional aluminum alloys (11). Due to high hardness, high thermal conductivity, low thermal expansion coefficient, wear resistance, impact resistance, corrosion resistance, low density, strength to weight ratio, relatively reasonable price and isotropic properties, these composites have many applications in various industries (11, 12). Reinforcements can be particles, layers, fibers or interpenetrating type. Also, according to the type of reinforcement, the composite can be classified into laminar composite, flake composite, fiber-reinforced composites, filled composite and particle-reinforced composite (10). Particle-reinforced composites are divided into two categories. In the first category, the heat treatment process leads to chemical reactions between the reinforcement phase and the matrix phase, which results in a homogeneous distribution of the stable reinforcement phase in the matrix. In the second category, reinforcement particles are embedded in a metal matrix, and the best way to make this type of composite is to use powder metallurgy (13, 14). Recently, the use of quasi-crystalline materials as reinforcement particles in aluminum-based composites has received much attention (15, 16), because quasicrystalline alloys and composites containing quasicrystalline phase improve some properties due to their complex atomic structure, unique mechanical and tribological properties, and special thermal behavior (17, 18). These properties make them suitable for applications such as surface coatings, reinforcement particles in composites and catalytic applications (4, 19, 20). Conventional sintering methods such as hot press, high temperature extrusion, hot isostatic press lead to grain growth which affects the properties of the final product. Spark plasma sintering (SPS) method is one of the techniques using powder metallurgy (21, 22). Compared to conventional sintering techniques, the SPS method can be very effective due to its unique sintering mechanisms. In this method, pressure and pulsed current simultaneously are used to achieve high density components (21, 23, 24). In the SPS method, momentary melting and evaporation on the particle surfaces leads to the formation of necks between the particles (22). When particles are in contact with each other, a high-density electric current passes through these particles, causing a bond between the particles. Uniaxial pressure also causes plastic deformation, which ultimately increases the density (25). Using this method, high density samples can be obtained at very low temperatures and times (26). Excessive interfacial diffusion can be avoided by using this method because the quasi-crystals exist only in a small composite range (27). Amini et al. (3) synthesized Al<sub>67</sub>Cu<sub>20</sub>Fe<sub>10</sub>B<sub>3</sub> quasi-crystalline alloys using mechanical alloving method. They studied the microstructural and structural evolutions of these materials at different times of the mechanical alloying process. Their results showed that the stable AlCuFeB single quasi-crystalline phase can be synthesized using high energy planetary ball milling in a short time from mechanical alloying process (around ~ 4 hours). Yong et al. (28) achieved the quasicrystalline phase using the method of mechanical alloying and heat treatment. Asahi et al. (29) and Tsai et al. (30) also synthesized the quasi-crystalline phase by mechanical alloving method. According to the findings of other researchers, the compositional range from 10 to 14 atomic percent of iron and 20 to 28 atomic percent of

copper is a very suitable range for the formation of icosahedral phase (4, 31, 32). In this compositional range, the peritectic reaction between  $\lambda$ 2-Al3Fe and  $\beta$ -AlFe(Cu) phases with the remaining molten liquid is reported to be the main reason for the creation of this quasi-crystalline icosahedral phase (4). The quasi-crystalline icosahedral phase in aluminum-copper-iron system has high hardness and low fracture toughness (33, 34). It is also reported that adding boron to this alloy system can significantly change the brittleness, hardness and toughness of these alloys (35, 36). In addition to these properties, boron causes more stability of the quasi-crystalline icosahedral phase and reduces the coefficient of friction and electrical resistance compared to alloys without boron (35, 37). Due to the special crystal structure and special properties, quasi-crystals have a wide variety of applications. One of the most important potentials of quasi-crystals is as a catalyst for steam-reforming of methanol (4). Also, quasi-crystals can be used in thermometry and heat flow detection due to their temperature-dependent electrical conductivity (4, 38). Another application of quasicrystals is light absorption. Thin layers of these materials are suitable as selective absorbers in solar thermal applications. These materials can also be used in glass and window applications, thermal insulation plates, and electrical insulation (4). In another research by Amini et al. [42] the effect of quasi-crystal on solar properties was investigated. In this research, they obtained a quick method for the synthesis of the quasi-crystalline phase, based on which there was no need for annealing operations and complex methods for the synthesis of the quasi-crystalline phase. Also, their results showed that the quasi-crystalline phase increased the amount of sunlight in solar. Addition of quasi-crystals to aluminum alloys leads to new properties in these materials. Lityńska-Dobrzyńska et al. (39) prepared aluminum matrix composites with Al<sub>65</sub>Cu<sub>20</sub>Fe<sub>15</sub> quasi-crystalline reinforcement phase with different percentages of the quasi-crystalline phase (20, 40 and 60 wt%). In order to prepare these composites, they used the hot vacuum pressing method. Their results showed that with increasing amount of quasi-crystalline phase, hardness and compressive strength of the composite increased (173 HV<sub>0.5</sub> and 370 MPa, respectively). They also reported that the friction coefficient of these composites depends on the composition (in the range 0.5-0.7). Sainfort and Dubost (40) used icosahedral Al-Li-Cu as reinforcement particles in the aluminium based MMCs. Tsai et al. (41) created composite material that contained quasi-crystals as reinforcement particles using powder metallurgy. It has also been shown that the hardness of this type of composite increased by increasing the quasicrystalline reinforcement particles up to 5 times compared to pure aluminum. Therefore, the use of quasicrystalline reinforcement particles in aluminum base composites has been proposed in order to overcome the low surface hardness of aluminum and increase the wear resistance of these materials (27). In this research, our goal was to synthesize A159Cu25.5Fe12.5B3 quasicrystalline compound using a new method without annealing and then to obtain Al/Al59Cu25.5Fe12.5B3 composite for the first time using SPS method. Also, according to the research of others, we realize that others use higher percentages of quasi-crystals as reinforcement, but considering that this project is a field for the industrial and practical use of quasi-crystals in the industry, from the volumetric percentages The bottom is used as reinforcement (5, 10, and 15) to investigate the effect on microstructure and mechanical properties.

### 2. MATERIALS AND METHOD

The raw materials of this research included Aluminum (purity percentage 99% < , particle size = 3 to 5  $\mu$ m), Copper (purity percentage 99.8% <, particle size = 14  $\mu$ m), Iron (purity percentage 99% < , particle size = 45  $\mu$ m > ) and Boron (purity percentage  $99^{-1}$ % < , particle size  $= 5 \,\mu m$ ) powders supplied by Aldrich company. Also, the Al<sub>59</sub>Cu<sub>25.5</sub>Fe<sub>12.5</sub>B<sub>3</sub> quasicrystal composition used in this study was prepared using the optimal research process by mechanical alloving method (42). Therefore, before the SPS process, first 4 samples were prepared according to the specifications of TABLE 1 and then the powders of quasicrystal and aluminum are mixed using ball-milling at 210 rpm for 4 hours. Composite samples of aluminum matrix were obtained by SPS method at a synthesis temperature of 320 °C and pressure of 20 MPa. Also, Figure shows a schematic of the process of sintering a bulk sample.

Phase analysis was carried out by a Philips MPD 1880 X-ray diffractometer (XRD) system with Cu-Ka radiation at 40 mA and 40 kV. The composition and microstructure of the sintered pellets were investigated by a JEOL JSM-5600LV field emission scanning electron microscope (FESEM), and Oxford energy dispersive spectroscopy (EDX) attachments with them. To evaluate the mechanical properties of the prepared samples, three-point flexural strength (Santam-STm 20) test was performed. It should be noted that three samples were used to reduce the measurement error for each test.

TABLE 1. Specifications of samples

Number	Combination					
1	Al					
2	$Al + 5 vol. \% Al_{59}Cu_{25.5}Fe_{12.5}B_3$					
3	$Al + 10 \ vol. \ \% \ Al_{59}Cu_{25.5}Fe_{12.5}B_3$					
4	$Al + 15 \ vol. \ \% \ Al_{59}Cu_{25.5}Fe_{12.5}B_3$					



Figure 1. Schematic of the process of sintering a bulk sample

#### **3. RESULTS**

Figure 2 shows for samples with different percentages of quasi-crystalline phase, there are only peaks related to the aluminum phase (cubic structure) as well as the quasicrystalline phase. Therefore, by performing the sintering process by SPS method, the peaks related to the quasicrystalline phase have not been eliminated and this phase has maintained its stability during the SPS process. In other words, in the SPS process, there is no interfacial reaction for this type of composite. It has been reported that in Al/Al-Cu-Fe composites, the ω-tetragonal phase is also formed due to the reaction between the quasicrystalline particles and the aluminum phase (43). However, as can be seen, the sintering process using SPS method has prevented the formation of  $\omega$  phase due to lower temperature and shorter sintering time. These results are consistent with the other researchers (27). Al/QC composites are stable in a large temperature regime and phase transformations occur at high sintering temperatures (43). With the occurrence of these phase transformations, the amount of quasi-crystalline phases also decreases. Kenzari et al. (44) concluded that the quasi-crystalline phase transformations to the  $\omega$  phase occur at approximately 450°C. It has also been reported that the reaction between aluminum and the quasicrystalline phase occurs at approximately 482 °C (43).

Figure 3 shows electron microscopy images for composites with different percentages of quasicrystalline phase. Also, Table 2 summarized the results of EDX elemental analysis from different regions (as shown in Figure 3). As can be seen for the sample with 5 vol% of the quasi-crystalline phase (region D in Figure 3 A), the amount of aluminum is equal to 68.03 at%, and the amounts of copper and iron are equal to 18.55 and 13.42 at%, respectively. Also, for samples with 10 and 15 vol% of quasi-crystalline phase, the amount of elements in regions D are very similar to samples with 5 vol% of quasi-crystalline phase. Therefore, the white areas (regions D in Figure 3) are related to quasi-



**Figure 2.** X-ray diffraction patterns for samples with different volume percentages of the quasi-crystalline phase in the aluminum matrix

crystalline reinforcement particles. In region E, for sample with 5 vol% of the quasi-crystalline phase (region E in Figure 3 A), the amounts of aluminum, copper and iron are 96.90, 1.98 and 1.12 at%, respectively. In regions E, the amount of the elements for samples with 10 and 15 at% of the quasi-crystalline phase are almost similar to samples with 5 vol% of the quasi-crystalline phase. Therefore, the dark gray areas (regions E in Figure 3) are related to the aluminum matrix phase. In region F, for the sample with 15 vol.% Of the quasi-crystalline phase (region F in Figure 3 C), the amounts of aluminum, copper and iron are 52.34, 0.33 and 0.31at%, respectively. As can be seen, reinforcement particles are scattered in the aluminum matrix. It can also be seen that the quasi-crystalline particles are agglomerated together. In addition to these elements, the elemental EDX analysis for this region also indicates the presence of the oxygen. For samples with 5, 10 and 15 vol% of the quasicrystalline phase, the amount of oxygen in the F regions are 39.61, 37.77 and 46.97at%, respectively. As shown in Figure 3, the F regions are mostly formed at the interface between the quasi-crystalline phase and aluminum. It is reported that at the interface between the quasicrystalline particles and aluminum, an amorphous oxide layer is formed in these composites, which acts as a strong bond between the quasi-crystalline particles and the aluminum matrix (27, 45). According to Figure 3, it is also observed that agglomerates of quasi-crystalline particles have formed in some areas. In addition, pores are observed in some areas, which can be due to the time of the mechanical alloying process and the temperature and sintering time.

The Flexural strength results of the pure Al sample and the samples with different percentages of the quasicrystalline phase are shown in Figure 4. Due to the fact that aluminum is a soft and ductile material, during the bending test, brittle fracture does not occur in this sample.



**Figure 3.** Scanning Electron microscopy images of composites with different percentages of quasi-crystalline phase A) 5vol.% of the quasi-crystalline phase B) 10vol.% of the quasi-crystalline phase and C) 15vol.% of the quasi-crystalline phase

**TABLE 2.** Results of EDX elemental analysis for samples with different percentages of quasi-crystalline phase

Samples	Phase areas	Al (at%)	Cu (at%)	Fe (at%)	0 (at%)
	D	68.03	18.55	13.42	
5vol.%	Е	96.90	1.98	1.12	
	F	59.42	0.53	0.44	39.61
10vol.%	D	68.46	18.02	13.52	
	Е	97.59	1.39	1.02	
	F	49.57	0.54	0.39	37.77
15vol.%	D	69.03	17.61	13.36	
	Е	98.69	0.73	0.58	
	F	52.34	0.33	0.31	46.97

However, in composite samples with different percentages of quasi-crystalline materials, it is observed that by performing the flexural strength test, the samples break brittle. And the fracture in these samples is of the brittle fracture type. Based on this, it is observed that composite samples do not have a plastic region, Accordingly, for the Al sample, the elastic region is examined and compared with other samples. It is observed that in the elastic region, the flexural strength for Al sample is about 47.30 MPa and for composite samples reinforced with 5, 10 and 15% of the quasicrystalline phase are 95.51, 146.83 and 192.92 MPa, respectively. Therefore, with increasing amounts of

reinforcing quasi-crystalline materials improve the mechanical properties (46). One of the factors affecting the final properties of composites is the interface between the reinforcing phase particles and the matrix phase. In such a way that a joint with strong adhesion leads to the distribution and transfer of force from the matrix to the reinforcing particles, which leads to an increase in modulus and strength. A suitable joint is created by the wetting of the particles by the liquid phase during the sintering process. Other factors affecting the final properties of the composite are the surface reaction at the interface of the reinforcing particles with the matrix phase. This reaction due to its products and factors such as the adhesion of reactive products to the matrix and reinforcing phase, thermal expansion coefficient and strength of reactive products, etc. can have a positive or negative effect on the mechanical properties of the composite (47). Also, the final mechanical properties of the composite are affected by the joint quality season of the reinforcing particles with the matrix phase, which depends on factors such as the adhesion of the phases in the composite, the thickness and amount of reaction products in the joint season, and so on (48).

The level below the applied load diagram in terms of displacement in the 3-point flexural strength test indicates the fracture energy, which is also a measure of toughness for the samples (48-50). Figure 5 shows the changes in applied load in terms of displacement in the flexural strength test of composite samples. Also, Table 3 presents the results related to the flexural strength of the samples. Therefore, it is observed that fracture energy, elastic modulus and stress increase with increasing amount of reinforcement in composite samples (51). But the percentage of elongation in the sample with 10% by volume is higher than other samples. In addition, it is observed that the amount of toughness in samples 10 and 15 is almost equal, while in the sample 15% of fracture energy, elastic modulus and stress is more than 10% of the sample.



**Figure 4.** Flexural strength changes in the elastic region for pure aluminum sample and samples with different percentages of quasi-crystalline materials



**Figure 5.** Load changes in terms of displacement in flexural strength test of samples with aluminum reinforcement reinforced with 5, 10 and 15 vol% quasi-crystalline

**TABLE 3.** Results related to flexural strength for samples with different percentages of quasi-crystalline phase

Sample	Stress (MPa)	Elongation (%)	Module (MPa)	Energy (J)	Elastic Module (MPa)	
2	14.74	2.72	541.91	90.63	144.71	
3	22.02	3.35	656.47	160.94	171.61	
4	29.90	3.31	953.39	210.92	296.70	

#### 4. CONCLUSIONS

In this research, the microstructural and mechanical properties of Al<sub>59</sub>Cu<sub>25.5</sub>Fe<sub>12.5</sub>B<sub>3</sub> composite samples synthesized by SPS method were investigated and the following results were obtained:

1. According to the XRD results, the quasi-crystalline particles maintain their stability due to the use of the SPS method and prevent the formation of the destructive  $\omega$  phase in the composite sample.

2. According to the FESEM images, with the increase of quasi-crystalline particles in the sample, in addition to the increase in dispersion, the accumulation of quasi-crystalline particles is observed in some areas, which may be due to short mixing or sintering temperature and time.

3. According to the Flexural strength results, due to the high hardness and excellent properties of the quasicrystalline particles, it is observed that by adding their amounts in the composite samples, it increases the fracture energy, stress and toughness. According to the obtained results, it is possible to investigate the practical use cases in the industry and their properties in the future research of quasi-crystals with volume percentages in this research. In addition, other properties such as corrosion and wear can be investigated for this research.

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# Persian Abstract

#### چکیدہ

در این مطالعه، کامپوزیتهای زمینه Al تقویتشده با ساختار شبه بلور AlsoCu25.SFe12.5B3 به روش تف جوشی پلاسمای جرقهای (SPS) تهیه شدند و خواص ریزساختاری و مکانیکی آن ها مورد بررسی قرار گرفت. مشاهده شد که با افزودن مقدار تقویت کننده شبه بلور، شدت پیک فاز شبه بلور افزایش یافت. همچنین با انجام SPS ذرات شبه بلور پایداری خود را حفظ کردند و به دلیل دمای پایین فرآیند و زمان کوتاه SPS فازهای مخرب در شبه بلور به وجود نیامد. علاوه بر این، با توجه به تصاویر میکروسکوپ الکترونی روبشی (FESEM)، توزیع ذرات شبه بلور در سطح نمونه افزایش یافت. خواص مکانیکی نیز با افزایش درصد حجمی شبه بلور به بلور به ورم می مود با ۱۵ درصد حجمی شبه بلور به دلیل خواص مکانیکی و ریزساختاری بهتر نسبت به سایر نمونه ها، به عنوان نمونه بهینه با خواص کاربردی مناسب انتخاب شد.



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# Experimental Study of Thermal Ageing and Hydrogen Embrittlement Effect on the Equipments of a Rocket Engine

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#### ABSTRACT

In the present study employed disc pressure tests to assess the effects of hydrogen embrittlement and thermal ageing on the fatigue life of a thin-wall circular part within a rocket engine. The technique compared the pressure resistance of membranes tested under helium and hydrogen, offering a simple, sensitive, and reliable method. Disc tests were selected to mimic natural operating conditions, as they align with those of a thin-wall circular part within a rocket engine. The originality of these tests appears to lie in their enhanced performance in terms of sensitivity and reproducibility. To achieve this, tests were conducted across various conditions, including sample thicknesses of 0.75 mm, a broad range of strain rates from  $10^{-6}$  s<sup>-1</sup> to  $10^{0}$  s<sup>-1</sup>, temperatures spanning from  $20^{\circ}$ C to  $900^{\circ}$ C, and pressure rates from  $10^{-2}$  to  $2.10^{4}$  MPa/min. Furthermore, a variety of materials were investigated, including copper, nickel alloy, and stainless steel. The results demonstrated that thermal aging leads to precipitation, particularly intergranular precipitation. These precipitates diminish the material's ductility, particularly when they are nearly continuous. Additionally, the material's sensitivity to hydrogen becomes significant when hydrogen, supersaturated due to rapid cooling, becomes trapped on precipitates formed at high temperatures. Furthermore, the results indicated that thermal and hydrogen-induced damage mutually reinforces each other, resulting in reduced fatigue life under high deformation.

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#### **1. INTRODUCTION**

Hydrogen embrittlement (HE) is a common and significant issue for various metallic materials. The challenges posed by hydrogen embrittlement are diverse, stemming from its introduction during material development, part manufacturing, and service stages. This occurs when the equipment comes into contact with hydrogen-containing gases or is exposed to hydrogen generated through corrosion, electrochemical processes, and water dissociation. The actual service environment constitutes an external factor influencing HE behavior, while the internal factor involves the accumulation of hydrogen atoms due to interactions with shallow hydrogen traps. Potential sites for these traps in martensitic materials include grain boundaries (1) and dislocations (2). Several studies have highlighted the pivotal role of hydrogen-dislocation interaction in local

hydrogen accumulation and plasticity (3, 4). This phenomenon can be accelerated through the hydrogenenhanced localized plasticity (HELP) mechanism, suggesting that trapped hydrogen in dislocations facilitates dislocation emission and movement (5).

For many metal alloys, mechanical strength, ductility, and fatigue life can be substantially reduced when exposed to hydrogen. Hydrogen-related brittle fracture becomes more intricate due to the interaction between hydrogen and stress under various loads. Wang et al.'s findings (6) demonstrated that the fracture strength of SSRT (slow strain rate tensile) at a rate of  $1 \times 10^{-7}$  s<sup>-1</sup> surpassed the threshold strength for CLT (constant loading tensile). Introducing nanoparticles into the matrix significantly enhanced the strength of DSHS (Dual-Phase Steel) without compromising its toughness and plasticity, as these nanoparticles served as effective irreversible hydrogen traps, mitigating HE risk (7).

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Qianqian et al. (8) studied the influence of adding Mo to Ti which was investigated concerning hydrogen-induced cracking behavior. They concluded that Mo addition affected the interaction between hydrogen, defects, and cracking behavior, offering insights into enhancing the hydrogen-cracking resistance of titanium alloys in structural materials. Additionally, Momotani et al. (9) revealed hydrogen accumulation at the prior austenite grain boundaries, particularly at lower strain rates ( $8.3 \times 10^{-6} \text{ s}^{-1}$ ). However, the impact of temperature on hydrogen accumulation and hydrogen-induced fracture remains unclear. Literature indicates increased hydrogen diffusion rates with rising temperatures (10), while hydrogen susceptibility initially increases and then decreases (11, 12).

Extensive research into metals' sensitivity to hydrogen has led to established solutions for specific contexts. However, evolving contexts and demands for enhanced material performance necessitate further exploration without compromising hydrogen resistance. Theoretical and bibliographical approaches aid in preselecting materials based on numerous embrittlement parameters, though accurate qualification through tests reflecting service conditions remains essential. To mimic these conditions, Shenguang et al. (13) systematically studied hydrogen embrittlement in 15Cr martensitic stainless steel used for steam turbine blades. Slow strain rate tensile (SSRT) and constant loading tensile (CLT) tests were conducted at room temperature and 80°C.

Notably, despite lower hydrogen concentration during SSRT, the hydrogen-induced fracture strength of 15Cr steel in SSRT was lower than the threshold for CLT due to enhanced local hydrogen concentration from mobile dislocation transport during SSRT. Moreover, even with higher hydrogen concentration absorbed during SSRT at 80°C, the hydrogen embrittlement susceptibility was lower due to reduced local hydrogen accumulation at higher temperatures.

Standard techniques for characterizing metals under hydrogen conditions fall short in simulating combustion chamber behavior subjected to on-off cycles. Rocket engines, for example, experience detrimental cycles where hydrogen content increases during hightemperature usage, remains trapped during rapid cooling upon shutdown, and leads to super-saturation-induced damage during low-temperature restart. This supersaturation can shorten material fatigue life.

Additionally, thermal ageing following medium to high-temperature usage leads to uneven growth of initial precipitates, especially near grain boundaries, resulting in metallurgical embrittlement. Such embrittlement amplifies when materials are employed in hydrogen-rich atmospheres. To effectively understand hydrogen embrittlement and thermal aging effects on rocket engine fatigue life, practical service conditions must be simulated in the lab. Monotonic biaxial tests, such as gas disc pressure tests on membranes loaded by internal gas pressure, offer advantages over traditional tensile tests by providing wider temperature and strain rate ranges. The interplay of load conditions and service temperature, alongside varying materials' susceptibility to HE, is pivotal during rocket engine service.

This article introduces a specific technique for characterizing metals under hydrogen conditions using disc testing. The aim is to uncover the impacts of thermal aging and hydrogen on rocket engine service life during on-off cycles while considering multiple parameters. Moreover, numerical results are presented to enhance awareness of hydrogen-related issues among designers and analysts. This technique surpasses conventional approaches to hydrogen embrittlement, especially for equipment under severe stress like rocket engines. Materials for such engines must demonstrate low hydrogen embrittlement across broad temperature ranges. Current research primarily focuses on studying hydrogen embrittlement degradation mechanisms and thermal aging to address long-term performance demands of rocket engines.

#### 2. MATERIALS AND METHODS

**2.1. Material** Three materials have been used in the present study:

**2.1.1.Low-alloy Copper (CuCrZr)** DLR provided a copper alloy (Cu-0.65%Cr-0.05%Zr), which is a material with structural hardening properties. It as-delivered state, the alloy underwent a solution treatment, followed by over-aging and precipitation tempering at 450°C. The alloy, after undergoing this treatment, offers a favorable balance between high thermal conductivity and improved mechanical characteristics.

**2. 1. 2. Nickel Alloy (Inconel 600)** Imphy provided Inconel 600, a nickel-based superalloy containing (14 to 17%) chromium and (6 to 10%) iron. The melting range of this alloy falls between 1350-1410°C. This alloy exhibits good high-temperature strength up to 1150°C and resists chemical corrosion at elevated temperatures. In terms of high-temperature engineering, the alloy demonstrates strong resistance to oxidation and carburization. Due to its versatility, Inconel 600 finds applications across various fields with demanding thermo-mechanical and chemical conditions, including the chemical industry, aeronautics, space, and nuclear reactors. The cold-rolled sheet is pickled and annealed at 970°C in a continuous furnace.

**2.1.3. Stainless Steel: AISI 321 Steel (14)** AISI 321 steel is also known as austenitic stainless steel due to its titanium content, which prevents corrosion. Type 321

cannot be hardened through thermal treatment, but its strength and hardness can be significantly increased by cold working, despite a reduction in ductility. Annealing: Heat it to 1750 - 2050°F (954 - 1121°C), then water quench or air cool.

The chemical composition, mechanical and thermal properties of the materials used are provided in Tables 1 and 2, respectively. It should be noted that for the copper alloy, chromium (Cr) and zirconium (Zr) contents adhere to the specifications, while other elements are present only in trace amounts.

#### 2.2. Presentation of the Disc Testing

**2.2.1. Experimental Procedure** The setup for the disc testing cell is illustrated in Figure 1. The disc testing employs a flat piece with a consistent thickness, closely resembling the thickness of the combustion chamber wall. The disc, embedded at its periphery, is subjected to increasing gas pressure on its bottom face, and the deflection at the midpoint of the upper face is measured. The pressurization rate remains constant throughout the usual rupture tests. The evolution of the gas pressure during the test exhibits three main steps, as illustrated in Figure 2:

- The transient loading period: This results from gradually opening the adjusting valve to achieve the desired gas flow.
- The steady increase in gas pressure: The curve's slope corresponds to the intended loading rate.
- The abrupt drop in gas pressure: This corresponds to the failure of the disc.

The influence of hydrogen on material properties can be measured by comparing results obtained with interstitial helium and deleterious hydrogen. Additionally, this disc testing method offers a wide range of strain rates (from  $10^{-6}$  s<sup>-1</sup> to  $10^{0}$  s<sup>-1</sup>) and temperatures (from 300K to 1200K); the prior heating duration is relatively short (about 1.5 hours).

The choice of material components for the disc testing cell depends on the testing temperature and the gas used (inert or harmful). An elastomeric O-ring (see Figure 3) is used for testing the material under inert gas at room temperature; at higher testing temperatures, a metallic O-ring (see Figure 4) must be employed. Because the loading gas should not be contaminated by gases occluded in the O-ring or permeating through the elastomer, the O-ring is also metallic during any environmental testing. The metallic O-ring is not

TABLE 1. Chemical composition of the materials studied (spectrum, wt, %)

Materials studied	С	Cu	Cr	Zr	Р	S	Ni	Al	Fe	Si	Ti	Мо	Mn
CuCrZr alloy	-	99	0.69	0.056	0.006	0.0013	0.006	< 0.002	0.007	< 0.005	-	-	-
Inconel 600	0.044	0.22	15.26	-	-	0.003	75.5	-	8.27	0.5	-	-	0.18
AISI 321 steel	0.08	-	19.00	-	0.04	0.03	12.00	-	remain	0.75	0.70	0.50	2.00

TABLE 2. Mechanical and thermal properties of the materials studied (as it is)

Materials studied	Young's modulus E [GPa]	Elastic limit σel [MPa]	Fracture limit σf [MPa]	Elongation A [%]	Thermal conductivity $\lambda$ [Wm-1K-1]	Coefficient of thermal expansion, α
CuCrZr alloy	120	255	370	18	320	18.10 <sup>-6</sup> /K
Inconel 600	207	352	693	36	14.9	13.3x10 <sup>-6</sup> /°C
AISI 321 steel	180	276	612	45	16.2	17.2 µm/m/°C



Figure 1. Schematic of the used disc testing cell



Figure 2. Typical evolution of the gas pressure during the disc testing



**Figure 3.** Standardized Elastomeric O-ring



**Figure 4.** Metal O-ring provided by Advanced Products

reusable. The sample and the cell can be heated by an annular resistor furnace. Both the cell and the furnace are insulated with ceramic fiber-based panels and stainless steel sheets (see Figure 7).

**2.2.2. Samples** The samples of disc testing are flat discs with constant thickness; the disc thickness is similar to the thickness of the combustion chamber wall to be close to the real material service conditions.

- The disc diameter is 58 mm (see Figure 5).
- $\blacktriangleright$  The disc thickness is 0.75 mm (see Figure 6).

**2. 2. 2. Disc Testing Equipment** As shown in Figure 7, the disc testing equipment consists of three main subsystems: the tightening system, the gas supply system, and data acquisition. The tightening pressure applied to the periphery of the bottom disc face is provided by a high-pressure hydraulic jack. The pressure amplifier ENERPAC AHB-46, shown in Figure 8, is the core device in the tightening system. This device amplifies the low air pressure (0.4 MPa) up to the high oil pressure (20 MPa), as illustrated in Figure 9. The relative air elasticity is crucial to ensure a nearly constant load on the disc periphery during thermal cycles and subsequent thermal differential deformations.

The gas supply system provides mechanical loading through gaseous pressure and the ambient atmosphere around the disc. Since hydrogen damage can be partially or fully masked if the hydrogen used is not sufficiently pure, adsorbed gases (particularly oxygen and water vapor from the initial ambient atmosphere) must be purged from the supply pipes and downstream volumes. Prior equipment rinsing is achieved through three cycles of alternating filling with pure gas at low pressure (0.1



Figure 5. Disc sample with a diameter of 58 mm



Figure 6. Flat disc with constant thickness of 0.75 mm

MPa) and vacuum pumping of the contaminated gas. The loading gas is sourced from a gas cylinder at very high pressure (up to 150 MPa), as shown in Figure 10.

Gas supply is regulated using opening and throttle valves depicted in Figure 11. Gas pressure is measured by a digital pressure sensor with a precision of  $\pm 0.1$  MPa. The deflection of the disc pole is measured using a Low Voltage Differential Transformer (LVDT) displacement transducer with a precision of  $\pm 10$  µm. Sample temperature is measured with a thermocouple on the upper disc face. All experimental data are monitored and recorded using a digital plotter (see Figure 12). The sampling period is short enough to capture data at a high rate.

**2. 3. Mathematical modelling of the disc mechanical properties** To calculate the plastic strain and stress at the pole of the disc from the measured deflection and pressure (15, 16), an analytical calculation similar to Hill's method (17) is employed. The calculation of plastic strains and stresses is based on the following assumptions: the stresses are biaxial because the



Figure 7. Schematic of the disc testing equipment





**Figure 8.** Air-oil pressure amplifier ENERPAC AHB-46

**Figure 9.** Hydraulic diagram of the pressure amplifier



Figure 10. Gas storage at high pressure Figure 11. Gas supplying



Figure 12. Data acquisition Digital plotter SEFRAM 8400

maximum axial stress is the gas pressure, which is negligible in comparison to planar stresses; the material is homogeneous and isotropic, and the volume of a metallic material remains constant during plastic deformation; the thin disc is deformed as a membrane, meaning flexion is neglected at the pole.

The most general mechanical loading involves 6 independent parameters: 3 principal stresses and 3 principal strains. For the disc loading, the axial stress is nullified; the Von Mises stress and strain are calculated from the remaining 5 parameters to facilitate the comparison of results between disc testing and tensile testing. While the Von Mises stress and strain are limiting factors due to the reduction of the disc behavior description from 5 initial parameters to 2, they have consistently enabled coherent comparisons of different mechanical loadings in various applications (18-21). The Von Mises stress and strain are determined from Equations 1 and 2.

Note: The Equations 1 and 2 are referenced in the text, but the actual equations themselves are not provided. Please make sure to include the equations if they are relevant to the context.

$$\bar{\sigma} = \frac{P.\rho}{2.t} \tag{1}$$

$$\overline{\varepsilon} = \ln(t_0 / t) \tag{2}$$

where : P is the gas pressure,  $\rho$  is the cupola radius at the disc pole, t is the pole thickness of the deformed disc and t<sub>0</sub> is the initial thickness of the disc.

If the deformed disk is assumed to be a spherical cupola, the pole radius  $\rho$  becomes the radius of the sphere. This radius is determined from the deflection W using the geometrical Equation 3 formulated for the outer fiber of the disc (refer to Figure 13). We have confirmed through dimensional measurements that the disc indeed deforms into the assumed spherical cupola.

$$\rho = \left(W^2 + A^2\right) / \left(2.W\right) - r \tag{3}$$

where : W is the deflection at the disc pole, A is the internal radius of the disc embedding and r is the die radius at the disc embedding.



Figure 13. Disc deformation-geometrical parameters

The strains at the disc pole are calculated from the deflection W by the analytic Equation 4 based on the above mentioned assumptions; this formula has been validated by measurements of the pole thickness obtained after the deformation of discs made of various materials,

$$\overline{\varepsilon_i} = 2.\int_0^{W_i} \underbrace{\left| 1 - \frac{2.r}{A} \cdot \left( \frac{1}{1 + W^2 / A^2} \right) \cdot \sin\left( 2.Arctg\left( \frac{W}{A} \right) \right) \right|}_{\rho} dW$$
(4)

where : W is the deflection at the disc pole, A is the internal radius of the disc embedding, r is the die radius at the disc embedding and  $\rho$  the radius of the disc deformed as a spherical cupola; the radius  $\rho$  is calculated from the deflection with the Equation 3.

Testing disc associated to the previous calculation method provides coherent mechanical properties, similar to the usual tensile mechanical properties.

The biaxial tests can be performed at temperatures between  $20^{\circ}$ C-900°C and at strain rates between  $10^{-6}$ - $10^{0}$  s<sup>-1</sup>; for instance, the tests can be performed at 900°C at high strain rate (22), which is difficult with another experimental technique.

2.4. Flowchart of Rocket Engine Damage Figure 14 depicts the flowchart of the rocket engine damage procedure, where the combustion chamber undergoes several 'Start-Stop' cycles, rapid cooling, rapid heating, and high temperature gradients, resulting in low cycle fatigue. Similarly, exposure to medium and high temperatures leads to thermal aging and subsequent low cycle fatigue. Furthermore, hydrogen embrittlement and its effects on low cycle fatigue occur. Additionally, the presence of trapped hydrogen contributes to embrittlement and super-saturation, reducing the material's lifespan. When the engine operates at high temperatures in a hydrogen environment, the material absorbs more hydrogen. During engine shutdown, rapid cooling prevents the hydrogen from escaping. Upon restarting, the material experiences plastic deformation at low temperatures and damage due to hydrogen supersaturation. Hydrogen supersaturation significantly reduces the material's lifespan. Another damaging factor



Figure 14. Flowchart of rocket engine damage

for the combustion chamber is the thermal aging of alloys resulting from frequent use at medium or high temperatures. These actions are taken to understand and clarify the impacts of hydrogen embrittlement and thermal aging on the fatigue life of a thin-walled circular part, which is a component of a rocket engine.

### **3. RESULTS AND DISCUSSIONS**

The results of disc testing are presented in order to reveal the influence of thermal ageing and hydrogen embrittlement on the fatigue life of rocket engines subject to on-off cycles.

**3. 1. Thermal Embrittlement** Thermal ageing is in two types, called stable and unstable thermal of alloys.

**3. 1. 1. Stable Thermal Alloys** For stable stainless steel, ductility increases at the highest temperatures when the rupture deflection increases (see Figure 15). For this alloy, the main phenomenon is the deflection drop at the intermediate temperatures (normalized T = 0.3 - 0.5); this light embrittlement is created by thermal ageing related to atom diffusion and consecutive precipitation; thermal ageing is relatively rapid during mechanical testing due to plastic deformation improves atom mobility; at intermediate temperatures, precipitation appears especially around the grain boundaries.

For the nickel alloy, Figure 15 shows that the fracture elongation changes minimally with temperature, as recrystallization and precipitation occur simultaneously, offsetting their effects. Micrographs confirm that holding at a sufficiently high temperature (T = 0.75 T melting) enhances intergranular precipitation, making it nearly continuous (see Figure 16). The heat treatment of the



Figure 15. Disc testing at different temperatures of stable thermal of alloys



**Figure 16.** Micrographs of the nickel alloy before and after testing at high temperature (results of Figure 15)

nickel alloy strengthens intergranular precipitation, rendering it almost continuous.

3. 1. 2. Unstable Thermal Alloys The tested copper alloy (see Figure 17) is initially treated by artificial ageing; this heat treatment at medium temperature gives fine, coherent and well-distributed precipitates, which increases mechanical resistance and decreases ductility. When the material is tested at temperatures higher than the ageing temperature (normalized  $T \ge 0.3$ ), the initial precipitates become coarser and less coherent with the matrix; this evolution is more important around the grain boundaries especially at the lowest temperatures; consecutive embrittlement may becomes very significant if the heating duration is long enough. Additionally, the precipitation modification increases the material ductility at normalized temperatures up to 0.35 and decreases the ductility for higher temperatures. The embrittlement increases if the heating duration increases.

For the nickel alloy as shown in Figure 17 is also unstable although it has not been treated by artificial ageing: for this material, the heating duration is great enough to obtain quasi continuous precipitates around the



Figure 17. Disc testing at different temperatures of unstable thermal of alloys

grain boundaries; under mechanical loading, these precipitates initiate inter-granular cracks and ruptures (see Figure 18). From grain to grain, the cracks propagate along the whole disc thickness and fine gas leakages appear; the leakages are detected by the mass spectrometer, while as they are very fine, the disc can be pressurized until rupture. The leakages are detected at relatively low deflection (see Figure 17); they characterize initiation of metal damage; obviously, tensile testing is not sensitive enough to detect such fine cracking and associate the initiation of damage.

**3. 2. Hydrogen Embrittlement** Hydrogen embrittlement includes two types: Gaseous and internal hydrogen embrittlement.

**3. 2. 1. Gaseous Hydrogen Embrittlement** The two presented cases are influenced on testing temperature and precipitation duration.

**3.2.1.1.Influence of Testing Temperature** The different effects of testing temperature as shown in Figure 19 illustrate:

- At lower temperatures, the copper alloy is hardly sensitive to hydrogen due to fine and coherent precipitates do not trap significant quantities of hydrogen,
- At medium temperatures, the precipitates become coarse and incoherent enough to trap hydrogen with the result that cracks are more easily initiated on the precipitates (23),
- At higher temperatures, the hydrogen embrittlement disappears because it cannot be trapped by the precipitates as it is very mobile.

Concerning the comparison with and without hydrogen, Figure 19 shows that at low temperatures the case without hydrogen is similar to that with hydrogen. However, at medium and higher temperatures the phenomenon observed without hydrogen is less intense than in the presence of this element, as shown by the relative arrow. Finally, in current study observes that this relative arrow decreases at higher temperatures in the case without hydrogen, conversely to the case with hydrogen.



**Figure 18.** Observations of tested discs (results of Figure 5); Nickel alloy tested at  $T > 0.5T_{\text{fmelting}}$ 



Figure 19. Disc testing at different temperatures of stable thermal of copper alloy

Concerning high temperatures, the value of the hydrogen content  $C_H$  in the engine wall reaches the hydrogen solubility  $S_H$  when steady state of diffusion has been reached. On this subject, Fick's equations give the theoretical time  $t_{\infty}$  to obtain the steady state when a thin wall is subjected to hydrogen on a single face (24):

$$t_{\infty} = 0.5e^2 / \mathrm{D}_H \tag{5}$$

where: e is wall thickness (e = 0.75 mm) and  $D_H$  is hydrogen diffusivity.

In the case of copper alloy, and to quote an order of magnitude, the steady state is obtained in about 40 s at the temperature of 900 K; however, at this example at high temperature a rocket engine is used during longer periods. During the steady state, hydrogen solubility  $S_H$  depends on the absolute temperature T (Arrhenius's law) and on the hydrogen partial pressure  $P_H$  (Sieverts's law),

$$S_{H} = S_{0} P_{H}^{1/2} \exp(-Q/R/T)$$
(6)

where:  $S_0$  is frequency factor;  $P_H$  is hydrogen partial pressure; T is absolute temperature; Q is activation energy and R = 8.31 Jmole<sup>-1</sup>K<sup>-1</sup>.

However, the hydrogen solubility in copper alloy is identical at 900 K under partial pressure  $P_{\rm H900}$  at 600 K under hydrogen pressure  $P_{\rm H600}\approx 450~P_{\rm H900}$  (25).

At 300 K, the hydrogen pressure  $P_{H300}$  would have to be much higher than that at 600 K to achieve the same hydrogen solubility. These calculations seem during service at high temperatures, a large amount of hydrogen is introduced into the engine walls; disc testing at room temperature must be performed under high gas pressure to introduce hydrogen into the material with content as high as during service at high temperature.

In addition, when the engine is stopped, it is rapid cooling kept hydrogen trapped on the precipitates that created at high temperatures. When the engine is restarted, high thermal gradients appear in the thin walls; these gradients create thermal strains in the material while it is super-saturated with hydrogen.

**3.2.2.1. Influence of Precipitation Duration** The thermal embrittlement of the nickel alloy strongly increases for the shortest ageing time (normalized t < 0.2) and its variation is less important for the longest ageing time (see Figure 20). Hydrogen embrittlement is almost identical at any ageing time and the hydrogen effect is added to thermal embritt1ement.

**3.2.2. Internal Hydrogen Embrittlement** Figure 21 shows the stable thermal of stainless steel where the hydrogen sensitivity determined at room temperature is almost identical without treatment (normalized T=0.18) or after heat treatment at medium normalized



Figure 20. Disc testing at  $20^{\circ}$ C after ageing treatments of Nickel alloy aged at T(K) > 0.5 melting temperature during t < tmax



**Figure 21.** Disc testing at 20°C after heat treatment of stable thermal of stainless steel

temperature (T = 0.4 - 0.5); the internal hydrogen embrittlement is identical to the gaseous hydrogen embrittlement.

For unstable thermal of stainless steel (see Figure 22), the internal hydrogen embrittlement is more important than for the stable alloy (Figure 21); at medium temperature, the precipitates of the unstable alloy have been modified and they become more efficient to trap hydrogen. For this unstable alloy, the internal hydrogen embrittlement seems more important than the gaseous hydrogen embrittlement; the precipitates trap more hydrogen during charging at medium temperature than during gaseous hydrogen testing at room temperature.

Precipitation evolution during thermal ageing is an important factor of hydrogen embrittlement. Discs tests under gaseous hydrogen may be slightly over-optimistic when they are used to characterize internal hydrogen embrittlement, consecutive to super-saturation during rapid cooling; this super-saturation may be simulated by internal hydrogen charging before mechanical testing.

Comparing Figures 9 and 10, we can say that Internal H embrittlement Unstable stainless steel > Internal H embrittlement Stable stainless steel => H trapping by precipitates (Int H  $\approx$  Gas H in the case of Stable stainless steel et Int H > Gas H in the case of Unstable stainless steel.

The disc testing method, used in conjunction with the previously mentioned calculation approach, yields consistent mechanical properties comparable to those obtained through conventional tensile testing. Both the ultimate strength and proof strength are identical, whether determined through disc testing or tensile testing. The mean values of uniform elongation are also the same for both methods, although there is relatively more significant scattering compared to strength scattering. This elongation scattering is influenced by local deformations initiated by material heterogeneities, such as surface defects (e.g., machining defects) and



**Figure 22.** Disc testing at 20°C after heat treatment of unstable thermal of stainless steel

metallurgical flaws (e.g., coarse inclusions). These heterogeneities induce area reductions that are detected with differing sensitivities in thick tensile specimens and thin discs. Furthermore, the outer periphery of the disc is not subjected to stress, preventing area reduction from edge defects, as observed in tensile specimens.

The mechanical properties are appropriately correlated with temperature and loading rate-dependent phenomena. At elevated temperatures, the strength of low-alloyed steel diminishes due to dynamic recrystallization during high-temperature deformation. At intermediate temperatures, the material experiences hardening attributed to solute atoms. Notably, hardening is more pronounced in disc testing compared to tensile testing due to distinct strain rates, a crucial hardening factor, in both specimen types.

Biaxial tests can be conducted within a temperature range of 20°C to 900°C and at strain rates from  $10^{-6}$  to  $10^{0}$  s<sup>-1</sup>. For instance, high-temperature, high-strain-rate tests can be performed at 900°C [26], a task that proves challenging with other experimental techniques. The aforementioned results underscore consistent comparisons between disc testing and tensile testing. As observed in other applications, the Von Mises stress and strain are sufficient for achieving coherent comparisons, even though they reduce the initial set of 6 stresses and strains to only 2 parameters.

**3.3. Low Cycle Fatigue** Figures 23, 24 and 25 show the influence of themal ageing, influence of gaseous hydrgen and influence of ageing and hydrogen of unstable Ni alloy respectely.



Figure 23. Low cycle fatigue : Influence of thermal ageing of unstable Ni alloy



Figure 24. Low cycle fatigue: Influence of gaseous hydrogen of unstable Ni alloy





Monotonic disc tests showed that the thermally unstable nickel alloy was weakened by thermal ageing and hydrogen. Disc fatigue tests revealed the same phenomena: service life was reduced by thermal ageing and hydrogen gas.

Service life is reduced more by hydrogen than by ageing; this result is logical since hydrogen embrittlement is higher than that obtained by ageing.

Disc fatigue shows the significant synergy between ageing and hydrogen embrittlement ; for a maximum fatigue strain of around  $10^{-2}$ , the life of a hydrogen-aged material is only 20 cycles, whereas it is around 10000 cycles if the material is damaged only by ageing or only by hydrogen.

When several on-off cycles are applied to the engine, its material subjected to low cycle fatigue; fatigue life may be reduced by the thermal embrittlement and by the hydrogen embrittlement; thus, the life reduction may be mutually amplified by both embrittlements. Fatigue results are not as detrimental for the alloys of rocket engines as for the prior nickel alloy but the phenomena may be similar; consequently, the phenomena must be identified and their influence on the fatigue life must be correctly characterized.

### 4. CONCLUSION

The various results obtained in the present study have led to the following conclusions:

- The fatigue life of rocket engines can be estimated through numerical calculations of damage; before conducting these calculations, both thermal and hydrogen damage must be correctly identified, characterized, and their mutual influence must be verified.
- There is significant synergy between degradation due to thermal aging and embrittlement caused by gaseous hydrogen, as the fatigue life is reduced from 10000 to 20 cycles in alternate fatigue tests at a deformation equal to 10<sup>-2</sup>.

- Thermal ageing primarily leads to precipitations around grain boundaries; intergranular precipitates reduce material ductility, particularly if they are nearly continuous.
- While hydrogen damage is minimal under usual service conditions, it might become unacceptable when hydrogen is supersaturated due to rapid cooling, remaining trapped on precipitates formed at elevated temperatures.
- Thermal and hydrogen damage mutually reinforce each other, significantly reducing fatigue life under relatively high deformation.
- In the nickel alloy, leaks occur at higher temperatures  $(T(K) > 0.5T_{melting})$  with deflections significantly lower than those obtained at rupture on the same sample.
- For thermally unstable stainless steel. embrittlement induced by hydrogen introduced before mechanical testing is more significant than that obtained under gaseous hydrogen.
- For reduced temperatures from 0.3 to 0.5, intergranular precipitation causes a loss of stainless steel ductility.
- Hydrogen sensitivity is sufficiently low when alloys are hardened by precipitates if they are fine, well distributed and coherent with matrix,
- The precipitate properties depend on chemical composition and thermal exposure consecutive to prior heat treatments or consecutive to services at medium and high temperature,
- The detection of very small leaks through the disc is useful to detect metallurgical evolutions of the material that create relatively short cracks while not changing the macroscopic mechanical properties.

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#### Persian Abstract

# چکيده

(i)

در مطالعه حاضر از آزمایش های فشار دیسک برای ارزیابی اثرات شکنندگی هیدروژن و پیری حرارتی بر عمر خستگی یک بخش دایره ای دیواره نازک در موتور موشک استفاده شد. این تکنیک مقاومت فشار غشاهای آزمایش شده تحت هلیوم و هیدروژن را مقایسه کرد و روشی ساده، حساس و قابل اعتماد ارائه کرد. آزمایش های دیسک برای تقلید از شرایط عملیاتی طبیعی انتخاب شدند، زیرا آنها با بخش دایره ای با دیواره نازک در موتور موشک هماهنگ هستند. به نظر می رسد اصالت این تست ها در عملکرد بهبود یافته آنها از نظر حساسیت و تکرارپذیری باشد. برای دستیابی به این هدف، آزمایش هایی در شرایط مختلف از جمله ضخامت نمونه ۲۰۰ میلی متر، طیف وسیعی از نرخ کرنش از ایها از نظر حساسیت و تکرارپذیری باشد. برای دستیابی به این هدف، آزمایش هایی در شرایط مختلف از جمله ضخامت نمونه ۲۰۰ میلی متر، طیف وسیعی از نرخ کرنش از داره ۲۰۱۲ - ۵۰ دماهای بین ۲۰ تا ۹۰۰ درجه سانتیگراد و فشار انجام شد. نرخ از ۲۰۱۰ تا ۲۰۱۶ مگاپاسکال در دقیقه. علاوه بر این، مواد مختلفی از جمله مس، آلیاژ نیکل و فولاد ضد زنگ مورد بررسی قرار گرفت. نتایج نشان داد که پیری حرارتی منجر به بارش، به ویژه بارش بین دانهای می شود. این رسوبات شکل پذیری مواد را کاهش می دهند، به ویژه زمانی که تقریباً پیوسته باشند. علاوه بر این، حساسیت ماده به هیدروژن زمانی قابل توجه می شود که هیدروژن، فوق اشباع شده به دلیل سرد شدن سریع، روی رسوبات تشکیل شده در دماهای بالا به دام می افتد. علاوه بر این، نتایج نشان داد که آسیب های حرارتی و ناشی از هیدروژن به طور متقابل یکدیگر را تقویت می کنند و در نتیجه باعث کاهش عمر خستگی تحت بند می شود.

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# Optimal Prediction of Shear Properties in Beam-Column Joints Using Machine Learning Approach

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#### PAPER INFO

# ABSTRACT

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Keywords: Joint Shear Strength Beam-Column Joint Reinforced Concrete Artificial Neural Network Shallow Feed Forward Model MATLAB The failure of shear-type beam-column joints in reinforced concrete (RC) frames during severe earthquake attacks is a critical concern. Traditional methods for determining joint shear capacity often lack accuracy due to improper consideration of governing parameters, impacting the behaviour of these joints. This study assesses the capabilities of machine learning techniques in predicting joint shear capacity and failure modes for exterior beam-column joints, considering their complex structural behaviour. An artificial neural network (ANN) model is proposed for predicting the shear strength of reinforced exterior beam-column joints. ANN, a component of artificial intelligence that learns from past experiences, is gaining popularity in civil engineering. The ANN model is developed using a dataset comprising material properties, specimen dimensions, and seismic loading conditions from previous experimental investigations. The model considers twelve input parameters to predict shear strength in exterior beam-column joints. Training and testing of the ANN model are conducted using established design codes, empirical formulas, and a specific algorithm. The results demonstrate the superiority of the proposed Shallow Feed Forward Artificial Neural Network (SFF-ANN) compared to previous approaches. The effectiveness of an Artificial Neural Network (ANN) model was quantitatively assessed in this study, with a focus on its performance in comparison to various design codes commonly used in structural engineering. The model was assessed using the coefficient of determination  $(R^2)$  and achieved R-squared values of 99%, 94%, and 98% during the training, testing, and validation stages, respectively. The study highlights the significance of beam reinforcement as a key element in estimating shear capacity for exterior RC beam-column connections. Although the proposed models exhibit a high degree of precision, future research should focus on developing improved models using expanded datasets and advanced algorithms for enhanced pattern recognition and performance.

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## **1. INTRODUCTION**

Beam-column joints are vital components of reinforced concrete moment resisting frames (RCMRF), and they are particularly susceptible to seismic loads as failure in these joints can result in the collapse of the entire structure (1). Extensive investigations following earthquakes have emphasized the significance of beamcolumn joints as they significantly influence the overall seismic performance of reinforced concrete (RC) frames (2). Beam-column joints play a crucial role in maintaining the structural integrity of the system. However, during strong seismic events, these joints may experience large deformations, leading to a reduction in their capacity to carry lateral and gravity loads. This can result in partial damage or even the complete collapse of the structure (3). In modern building design, joint shear failure is a common type of failure observed in beamcolumn joints.

This failure mode often occurs because the joints were not designed to withstand the anticipated loads based on the capacity design principles recommended in contemporary seismic codes. Shear failure in beamcolumn joints, even at relatively low deformations, is a

brittle failure mode that can potentially trigger a building's collapse (4). Given the critical role of beamcolumn joints and their vulnerability to seismic forces, it is imperative to properly design and reinforce these joints to ensure the overall safety and integrity of structures in seismically active regions.

Determining the dimensions of the strut and cut-point regions, which are crucial for predicting the shear strength of beam-column joints, presents a significant challenge when using the Strut and Tie Model (STM) (5). The shear strength of the joint plays a vital role as the beam-column joint can become a weak link if it is not adequately considered. Previous research has employed various individual-type machine learning (ML) algorithms, such as ANN-PSO, SVM, XGBoost, and decision trees, for predicting the shear strength of reinforced concrete joints (6). Among these techniques, ANN, GEP, and fuzzy logic-based evaluations of cement strength have shown promise as efficient ML-based prediction techniques for engineering structures (7).

The resisting mechanisms provided by the beamcolumn joint are fundamental in enabling RC-framed buildings to withstand seismic excitations (8). In predicting the shear strength of RC joints, the deformation of Type 2 joints indirectly informs the prediction of member shear strength and follows the conservative approach recommended by ACI 352-R02 (9). Before the adoption of "earthquake-resistant" structural design in the late 1970s and early 1980s, many buildings were primarily designed to carry gravity loads, lacking sufficient shear strength, flexural capacity, and flexibility to resist strong seismic ground motions (10). In the design and seismic analysis of tall structures, lateral load-resisting systems like RC shear walls are commonly utilized. Accurately predicting the capacity of these systems is a critical aspect of the design process (11). Predicting the capacity becomes complex due to the reinforcement characteristics of concrete and the interactions between flexure and shear. Furthermore, the response of the structure during seismic activity can influence the behaviour of the joint (12).

The limited lateral force-carrying capacity of beamcolumn joints is influenced by the material properties used during the structure's construction, which in turn impact the overall response of the structure (13). To ensure structural safety and prevent shear failure, it is crucial to accurately forecast the shear strength of RC beam-column joints in the design process (14). With the advancement of Artificial Intelligence in recent years, there has been a paradigm shift towards applying machine learning (ML) methods for predicting the shear strength of beam-column joints (6). As part of this trend, the present research aims to analyze the shear strength prediction of beam-column joints using a neural network tool in MATLAB.

## 2. LITERATURE SURVEY

For the forecast of outer beam-column joint shear capacity, Alagundi and Palanisamy (2) proposed using an artificial neural network. The simulations show that the suggested model of the neural network can predict the Exterior Beam-Column joint's shear strength. There are three effective artificial neural network methods, radial basis function neural network (RBFNN), backpropagation neural network (BPNN) and generalized regression neural network (GRNN) Zhang et al. (15) suggested identifying the failure modes and shear strengths. With the results, the testing and training phases are compared, which prove that both GRNN, BPNN and RBFNN models are powerful approaches for predicting the mode of failure and shear strength. By using ANN, Gene Expression Programming (GEP) and Network-Based Group Method of Data Handling (GMDH-NN) Naderpour et al. (16) predicted shear strength. The simulation confirms the ability of the patterns expected by, GMDH-NN, GEP and ANN which are appropriate for use as a tool in forecasting the concrete shear walls with high accuracy and shear strength. For the forecast of shear strength an artificial neural network model was proposed by Alagundi and Palanisamy (17) in the Joint of reinforced concrete exterior BC joints are themed to seismic loading; thus, the proposed ANN model can be used. For estimating the reinforced concrete shear strength, the beam-column is subordinated to regular load Marie et al. (6) proposed a framework. The simulation also reveals that the shear strength of the joint was predicted by using the Kernel regression, where the experimental values are closer than the joint shear strength which is predicted by using the parametric equation. Detailed methodologies and discussions of the two disciplines were presented by Marcos and Silva (3). Powerful digital technologies and computer systems showed dominance by presenting the regression and performance analysis through different trained neural network models.

To determine the RC beam-column joints stochastic shear strength Yu et al. (18) employed, the GPR algorithm. The simulations show that the kernel can efficiently enhance the generalization performance and prediction accuracy of the GPR Truong et al. (19) presented the Bayesian optimization (BO), BO-XGBoost hybrid model and extreme gradient boosting (XGBoost) algorithms was made and its hyperparameters were improved based on a collection of data of 320 test specimens. The suggested model exposed that the beam width, effective depth, tension reinforcement ratio, shear span-to-depth ratio and concrete compressive strength are crucial to the deep beams' shear strength. Zayan et al. (20) presented the ANN model offered a more accurate tool to compute R and capture the impacts of five primary parameters: steel reinforcement ratio, concrete compressive strength steel yield strength, steel fibre aspect ratio fibre and volumetric ratio given from trial data. The gathered results show that the first significant argument is the compressed power of the concrete. Al-Bayati (21) introduced a numerical pattern for the calculations of shear strength in the exterior and interior reinforced concrete beam-column joints that are subordinated to seismic loads. The results of 110 exteriors and 105 interiors of beam-column joints gathered from the literature, the fresh pattern is gauged. This research study contributes to the shear strength of the beam-column joint and its prediction using artificial neural networks.

Mabrouk et al. (22) evaluate the effect of using different shear reinforcement details on the punching shear behaviour of interior slab column connections. A comprehensive experimental program is conducted on sixteen specimens having the same concrete dimensions of  $1100 \times 1100 \times 160$  mm where the slab depth is chosen to be less than that stipulated by different design codes. The parameters under examination were the type of shear reinforcement arranged in a cross shape perpendicular to the column edges (single leg, multi-leg, and closed stirrups), the spacing between stirrups (25 and 50 mm), and the extended length covered by the stirrups (300 and 425 mm). Experimental results showed that slabs reinforced with multi-leg or closed stirrups, even for slabs with a thickness of 160 mm, had an increase in the shear capacity by up to 40% depending on the stirrup amount. A noticeable enhancement in ductility was also observed.

Singh and Sangle (23) presented a nonlinear static response of a vertically oriented coupled wall subjected to horizontal loading. The 3-storey vertically oriented coupled wall interconnected with coupling beams is modelled as solid elements in a finite element (FE) software named Abagus CAE and the steel reinforcement is modelled as a wire element. For the simulation of concrete models, a concrete damaged plasticity constitutive model is taken into consideration in this research. Moreover, with the help of concrete damage plasticity parameters, the validation of two rectangular planar walls was executed with an error of less than 10%. Finally, these parameters are used for modelling and analyzed the static behaviour of coupled walls connected with coupling beams. Furthermore, the maximum unidirectional horizontal loading helped in obtaining the compression and tensile damage as well as scalar stiffness degradation.

Sfaksi et al. (24) concern a numerical study of the behaviour of reinforced masonry (RM) structures under seismic loading. These structures are made of small hollow elements with reinforcements embedded in the horizontal joints. They were dimensioned according to the rules and codes commonly used. They are subject to vertical loads due to their weight and to horizontal loads due to seismic forces introduced by the accelerograms. The software used is the non-linear analysis program Drain2D, based on the finite element method, where the shear panel element was introduced. A series of calculations were performed on several structures at different levels, excited by three major accelerograms (El Centro, Cherchell, and Kobe). Throughout the study, our main interest was to evaluate the behaviour factor, ductility, and failure mode of these structures while increasing the intensity of earthquakes introduced. The results of this present study indicate that the average values of the behaviour factor and the global ductility were of the order of  $q \approx \mu \approx 3.00$ . The reinforced masonry structures studied have been broken by interstage displacement.

The literature review provides valuable insights into the use of various techniques for predicting shear strength in beam-column joints. Several authors have proposed the application of artificial neural networks (ANN) to forecast the shear strength of exterior beam-column joints (2, 17). Different types of ANN models, including radial basis function neural network (RBFNN), backpropagation neural network (BPNN), and generalized regression neural network (GRNN), have shown promising results in predicting failure modes and shear strengths. Furthermore, other researchers have explored the effectiveness of machine learning algorithms such as gene expression programming (GEP) and network-based group method of data handling (GMDH-NN) in predicting shear strength (16). The application of these techniques, along with ANN, has demonstrated high accuracy in forecasting concrete shear walls and their shear strength.

Additionally, studies have utilized techniques like kernel regression, Bayesian optimization (BO), and extreme gradient boosting (XGBoost) to determine the stochastic shear strength of RC beam-column joints (3, 6, 18, 19). These techniques have shown improvements in prediction accuracy and generalization performance. Moreover, the use of artificial neural networks (ANN) has proven to be an accurate tool for computing shear strength, considering various parameters such as steel reinforcement ratio, concrete compressive strength, steel yield strength, steel fibre aspect ratio, and volumetric ratio.

Furthermore, studies have examined the behaviour of vertically oriented coupled walls under horizontal loading (23). Nonlinear static response analysis, incorporating concrete damaged plasticity constitutive models, has been conducted to assess the behaviour of these structures. The analysis includes the evaluation of compression and tensile damage, as well as scalar stiffness degradation. Lastly, a numerical study explores the behaviour of reinforced masonry structures under seismic loading (24). The study investigates the effects of vertical and horizontal loads on these structures, with a focus on behaviour factors, ductility, and failure modes. Results indicate that the average values of the behaviour factor and global ductility are approximately 3.00, and the reinforced masonry structures exhibit failure due to interstage displacement.

In conclusion, the literature review presents a diverse range of approaches and techniques employed to predict shear strength in beam-column joints and analyzed the behaviour of related structural elements. These studies contribute to the advancement of knowledge in this field and provide valuable insights for designing safer and more resilient structures.

# 3. RESEARCH PROBLEM DEFINITION AND MOTIVATION

Flexural strengthening garnered the majority of attention than shear strengthening in RC beams and it has received very little research. Particularly dangerous are structures exhibiting brittle failure to shear force. Shear, a sudden, unexpected structural collapse mechanism is mostly caused by this. Deep beams are subject to shear force, which has a shear span to effective depth proportion (a/d) smaller than two. The behaviours of a deep beam exposed to vertical static stress differ significantly from those of a narrow beam in both the analytical approach and design. Because of the fast and brittle fracture of RC beams caused by shear action and the absence of logical design formulas in building regulations, the behaviour and design of RC beams under shear remain a source of worry for structural engineers.

The deformations that beam-column connections experience under earthquake loading have a substantial impact on the seismic behaviour of reinforced concrete structures. Some locations fail before they should under powerful earthquakes if they are not properly planned. The researchers show several variables, such as column and beam dimensions, joint transverse reinforcement yield strength, concrete compressive strength, volumetric joint reinforcement ratio, beam longitudinal reinforcement ratios, beam eccentricity, and column axial load, affect joint shear strength. The shear strength of joint elements makes it challenging to forecast the connection between beams and columns. Machine learning (ML) approaches are being used to forecast the beam-column joint's shear strength of connections as a result of the recent advancements in AI. Shear strength is crucial while applying ML to forecast joints. Based on the outcomes of earlier experiments, the most crucial variables that impact shear strength joint were selected to develop a parametric equation to predict joint shear strength.

## The Objective of the Study

- To study how different parameters impact beamcolumn joints' shear strength.
- To prepare data from pre-existing literature to model a neural network in MATLAB.
- Using prepared data Neural Network Model was trained and tested in MATLAB.
- To compare the analytical results extracted from MATLAB with experimental results from Pre-Existing Literature.

## 4. PROPOSED RESEARCH METHODOLOGY

Failure in shear is a sort of brittle failure with no warning signs, hence numerous studies have been conducted in the literature. To reduce shear failure in design techniques and preserve structural safety, it is crucial to properly forecast the strength of the RC beam-column connections. This problem can be resolved by using ML techniques, such as ANNs, as reliable modelling tools for calculating the shear strength of the joint and its connections in the beam-column. ANNs give patterns for a variety of artificial and natural phenomena, many of which are difficult to model using conventional parametric techniques. Consequently, the article proposed using Artificial Neural Network (ANN) with Shallow Feed-Forward (SFF) architecture for estimating the strength of exterior RC beam-column connections was subsequently proposed in the article. The block diagram of the proposed method is shown in Figure 1.



Figure 1. Block Diagram of the Proposed Work

A better understanding of the variables influencing the shear strength joint of connections in beam-column can be achieved by using machine learning analysis to look into the significance of input variables. This could result in the recommendation of useful potential methods for exploratory studies and the facilitation of lab experiments. The provisions for estimating joint shear strength for the six national codes viz., EN 1998-1:2004 (European Code EC-8), CSA A3.3:2004 (Canadian Code), IS 13920:2016 (Indian Code), NZS 3101-1:2006 (New Zealand Code), ACI 318-14 (American Code), and AIJ:2010 (Japanese Code) have been compared and evaluated in the current study using 13 experimental findings gathered from the literature. The aforementioned codes recommend different limitations on the parameters viz. confinement of joint by the effective joint depth, eccentricity between beam and column, beams, concrete compressive strength, and effective joint width. An investigation of the parameters' effects on joint shear strength revealed significant discrepancies between the code projections. The methodology equates forecast joint shear strength values with known experimental results to provide a credible design strategy.

4. 1. Experimental Program The primary objective of this study is to examine the periodic behaviour of exterior beam-column joints in reinforced concrete structures. To train, test, and validate the neural network, data sets have been prepared using experimental studies conducted by various researchers. The shear strength of these external beam-column joints is influenced by multiple factors, and a suggested approach involves utilizing an artificial neural network to predict this strength. Key inputs for the ANN model include the compressive strength of the concrete, the supports at the bottom and top of the beam, the beam-to-column depth ratio, the beam bar index, the depth and width of the joint, the yield strength of the linear support in the beam, the column load index, the joint shear reinforcement index, and the length of the beam. To assess the performance of the neural network, statistical measures such as the coefficient of correlation, root mean square error, and scatter index are employed.

In Figure 2, a typical exterior beam-column connection in an RC frame is illustrated. This region of the frame, where the beam and columns intersect, is subjected to both gravitational and lateral loads, resulting in significant shear forces, axial forces, and bending moments. The analysis considered the coupling between the beam and column in this joint region, taking into account these various forces. The beam's flexural capacity within the reference joint subassembly, as determined by geometry, reinforcing details, and material parameters, was estimated to be approximately 75 kN at the point of yielding for the longitudinal reinforcement. The dimensions of the concrete beam and column were assumed to be 230mm×230 mm, with a concrete grade of M25, while the axial load applied to the column was considered to be 1000kN. All other relevant factors were obtained from the respective codes and standards.

4. 2. Parameters Affecting Joint Behaviour Previous experimental findings have highlighted the substantial influence of material strength, both in steel and concrete, on the shear capacity of beam-column joints. Additionally, the level of confinement plays a crucial role in determining the behaviour of these joint systems. Confinement can be provided through cross supports within the joint or by incorporating the framing of cross beams and slabs into the linking area. The adequate constraint of the joint core is necessary to effectively transfer shear forces, anchor the beam reinforcement, and transmit the axial load of the column. To assess the degree of confinement, the volume of cross support in the connection region is calculated and then divided by the core volume, gross volume, or the effective volume for a single layer of transverse reinforcement. This computation yields the volumetric confinement ratio. The ratio that exhibits the strongest correlation with the results is identified as a significant contributing factor in determining the joint's strength.



Figure 2. Geometry and Reinforcement Details (Dimensions in mm)

Furthermore, several additional parameters have been identified as influential factors impacting the shear strength of the joint. These include the eccentricity between the longitudinal beam and column center lines, the sizes of the column and beam, and the magnitude of the axial load applied to the column. Consideration of these parameters is essential for a comprehensive understanding of the joint behaviour and shear strength.

To evaluate the influence of different parameters on joint shear strength, a correlation coefficient is employed as defined in Equation 5. In this statistical approach, the independent variable x represents various parameters, while the dependent variable y represents the joint shear strength. Establishing a direct comparison between shear strength and each variable, this gain insights into their relationship. It is important to note that these correlation provide approximate estimations of the values parameters' impact on shear strength, as the correlations are expected to exhibit nonlinearity. While there may be correlations among the individual parameters, this analysis does not consider cross-correlations. The primary objective at this stage is to understand the degree of association between the parameters and joint shear strength. Interestingly, the results indicate that the joint geometry has a relatively minor influence compared to the reinforcement ratio and axial load, which exhibit high correlation coefficients. This finding highlights the significance of the reinforcement ratio and axial load in determining joint shear strength.

$$Correlation(x, y) = \frac{\sum (x - \bar{x}) \cdot (y - \bar{y})}{\sqrt{\sum (x - \bar{x})^2 \cdot \sum (y - \bar{y})^2}}$$
(1)

The important variables that might be taken into account in the joint strength prediction are chosen when the correlation coefficients are achieved. Concrete compressive strength and volumetric joint reinforcement ratio, which shows the confinement given by the transverse reinforcement, are the two most important criteria, as was previously mentioned. As a result, values for the spacing, joint core, gross area, number of transverse reinforcing layers, and stirrup area are obtained. According to the following equations, the volumetric transverse reinforcement ratio can be calculated in three different ways by using the joint core volume, the effective confined amount as the gross bond volume and the efficient volume contains one covering of joint transverse reinforcement.

**4. 2. 1. RC Beam-Column Joint Modelling** The shear and compression acting forces for a typical external RC beam-column junction under seismic load are depicted in Figure 2. In the joint  $\operatorname{core} V_{jh}$ , the flat joint shear force can be calculated as follows:

$$V_{jh} = T_b - V_{c1} \tag{2}$$

where:

$$T_b = A_{sb} \cdot f_b \tag{3}$$

where,  $A_{sb}$  and  $f_b$  represent the area and stress of the longitudinal reinforcement of the beam, respectively,  $V_{c1}$  represents the horizontal shear of the column above the joint, and  $T_b$  illustrates the tensile force in the beam longitudinal reinforcement. The following formulas are used to compute the column shear above the joint, the beam shear $V_b$ , and the beam flexural moment  $M_b$ .

$$V_b = \frac{A_{sb}f_b j_{bd}}{L} \tag{4}$$

$$M_b = V_b \cdot L \tag{5}$$

$$V_{c1} = \frac{L + h_c/2}{H} V_b \tag{6}$$

where, *H* is the height of the column, which is equal to the height between the upper and lower column inflexion points, *L* is the length from the beam's inflexion point to the column's face,  $h_c$  is the total height of the column cross-section, and  $j_{bd}$  is the internal moment arm of the beam cross-section, which can be calculated as follows:

$$j_{bd} = h_b - \frac{x_b}{3} - \delta_{sb} \tag{7}$$

In Equation 7,  $h_b$  is denoted as the breadth of the beam,  $x_b$  for the intensity of the contraction zone in the beam cross-section, and  $\delta_{sb}$  for the distance between the closest edge of the beam cross-section and the centroid of the tensile beam reinforcement. By imposing the equilibrium of the internal forces on the beam after confirming that the concrete in compression remains within the elastic range, the value of  $x_b$  can be derived, which leads to:

$$\frac{b_b x_b^2}{2} + (A_{sb} + A'_{sb})n_{h,b}x_b - (A_{sb}d_b + A'_{sb}\delta'_{sb}n_{h,b} - A'_{sb}\delta'_{sb} = 0$$
(8)

where,  $\delta'_{sb}$  is the distance from the centroid of compressive beam reinforcement to the closest edge of the beam cross-section,  $b_b$  is the thickness of the beam cross-section at the face of the column,  $A'_{sb}$  is the area of longitudinal compressive reinforcement,  $d_b$  is the efficient breadth of the beam cross-section, and  $n_{h,b}$  is the modular ratio given by:

$$n_{h,b} = \frac{E_{sb}}{E_c} \tag{9}$$

where,  $E_c$  is the concrete elastic modulus, which can be assumed to be 4700 MPa if its value is not specified, and  $E_{sb}$  is the reinforced elastic modulus of the beam reinforcement. The following method is used to compute the joint shear.

$$M_b = P(L+d^1) \tag{10}$$

where, *P* is the failure load (N), *L* is the distance from the load's application point to the column's face (mm), and  $d^1$  is the cover (mm). The strain in the tensile support of

the beam is given a value. The process is terminated, if the moment produced by the force in the beam tensile reinforcement equals the moment computed in Equation 10. If not, the assumed strain is raised gradually until the moment equals the moment specified in Equation 11. The elastic modulus of the reinforcement was estimated to be 200 GPa. The formula for shear strength joint is represented as follows:

$$V_j = T_b - V_{col} \tag{11}$$

where,  $T_b$  is the tensile force in the beam longitudinal reinforcement (N),  $V_{col}$  is the force of the shear in the upper column (N), and  $V_i$  is the joint shear force (N).

**4. 3. Artificial Neural Network (ANN) Model for Shear Strength Prediction** Artificial Neural Networks (ANN) is a computational framework inspired by the learning process of the human brain. In the human brain, information is received and stored in the connections between neurons, forming a complex network. Similarly, an ANN consists of interconnected artificial neurons that can process and store information. The main goal of an ANN is to establish a relationship between input data and corresponding output, similar to how the human brain recalls information from its network of neurons. Through training, an ANN modifies its internal components to learn from the input-output patterns presented during the training process.

Once trained, an ANN can be used as a prediction model for new inputs that were not part of the training dataset. It uses the learned information from the training phase to make predictions for the missing data. However, the accuracy of these predictions is a crucial concern. To address this issue, the available data is divided into two parts: a training set and a testing set. The ANN is trained using the training set, and the predictions made by the model are compared with the known output values from the testing set. High performance in the testing phase indicates a reliable prediction model that generalizes well beyond the training data, avoiding overfitting. However, optimizing the weights in ANNs with multiple hidden layers can be challenging due to issues like vanishing gradients and convergence to local minima. Even with large datasets, these problems can limit the performance of ANNs with deep architectures, posing a bottleneck in their optimization process.

**4. 3. 1. Shallow Feed Forward Neural Network** Neural network fitting occurs when a series of neurons, connected through activation functions, are accumulated. During the training of a neural network, the coefficients of the activation functions in each neuron are gradually optimized. The adjustment of biases and weights is performed to establish a relationship between the input and output values provided in the training dataset. The performance of the network is evaluated using an error function, such as mean squared error, which compares the neural network's response to the training objective. To facilitate learning during the training process, backpropagation algorithms are commonly employed. These algorithms update the weights (w) and biases (b) of each neuron in a way that minimizes the performance function (error). This minimization process involves propagating the output error backwards from the output layer to the hidden and input layers, adjusting the weights and biases accordingly.

For this work, an SNN pattern with an easy form and ideal performance containing a hidden layer and an output layer was used. Among these, the hidden layer has several neurons, whereas the output layer just has one. Figure 3 depicts the topology of the SNN model. Each output of the neuron in an SNN model's hidden layer can be described as Equation 12.

$$y_i = \sum_{i=1}^N w_i x_i + b_i \quad (i = 1, 2, \cdots, i \le N)$$
(12)

where,  $y_i$  denotes the neuron's output, N is denoted as the whole value of the hidden layer's neurons,  $w_i$  and  $b_i$ stand for the  $i_{th}$  neuron's weight and bias, respectively; and  $x_i$  stands for the input data, which is made up of  $x_1, x_2, \cdots$ , and  $x_n$ . The hidden layer's neurons perform a nonlinear transformation on the input signal  $x_i$  to create the output signal $y_i$ . The activation function within the secret covering is the Sigmond nonlinear function $\sigma(x)$ , which is not readily divergent and is simple to derive during the transfer process. It can be expressed as follows:

$$\sigma(x) = \frac{1}{1+e^{-x}} \tag{13}$$

The system can obtain the creation of the SNN model as shown in the equation according to the topology of the SNN model.

$$Y = W \sum_{i=1}^{N} \sigma \left( \sum_{i=1}^{N} w_i x_i + b_i \right) + B = W \sum_{i=1}^{N} y_i + B$$
(14)

where, W and B represent the output layer's weight and bias, respectively. The output value Y of the SNN pattern can be produced after linear transformation from the output signal  $y_i$  of each hidden layer in the neuron, which is transferred to the output layer. The output layer's activation function is the linear function. The Mean



Figure 3. Shallow Neural Network Topology

Squared Error (MSE), whose minimal value denotes the best curve fit for the dataset, is used to determine when the function ends during training. To compare the MSE of the output value of the SNN pattern Y with the test data  $\hat{Y}$ , the weights and biases of the neurons inside the hidden and output layers are changed. Iterative training learning using the error descent along the gradient direction method is used to determine the model parameters corresponding to the minimum root of the MSE.

**4. 4. Database Collection** The effectiveness and validity of the proposed model in the training process rely significantly on the quantity and quality of the data available. To ensure reliable results, a comprehensive database of reinforced concrete joint tests has been meticulously compiled. The database includes detailed information on geometric dimensions, material properties, specific configurations, and the stress-strain history of the specimens.

The data collection process focuses on gathering testing results from various references, specifically targeting specimens with plain reinforced concrete. These specimens cover a wide range of parameters, such as different amounts of joint, beam, and column reinforcement, diverse material characteristics, varying column axial loads, eccentricities, and transversely framed beams. It is important to note that retrofitted specimens have been excluded from the database to maintain consistency and relevance.

Table 1 in this section summarized the results of 120 specimens tested by Hanson et al. (25), Karayannis et al. (26) and Salim et al. (27). In all of these experimental studies where joints in beam-column are subordinated to monotonic or cyclic load until one of the collapse types of failure in the joint or beam yielding followed by joint failure is presented.

				-		1 <b>1</b> Du		meetion							
Investigator		fc', ksi	fyc, ksi	fyb, ksi	Lb, in.	hb, in.	bb, in.	ρ	ρ'	Lc, in.	hc, in.	bc, in.	ρς	P/fc' Ag	γj TEST
Hanson et al. (25)	Specimen ID	3.3	64.8	51	120	20	12	0.02	0.01	137	15	15	0.05	0.86	11.6
	Unit 3	4.9	68.1	66.5	63	16	16	0.02	0.02	166	16	16	0.02	0.1	10.8
	Unit 4	4.9	68.1	66.5	63	16	16	0.02	0.02	166	16	16	0.02	0.25	12.4
Pantelides et al. (28)	Unit 6	4.9	68.1	66.5	63	16	16	0.02	0.02	166	16	16	0.02	0.25	11.7
	Unit 5	4.6	68.1	66.5	63	16	16	0.02	0.02	166	16	16	0.02	0.1	10.4
	BS-L	4.48	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	8.13
	BS-U	4.5	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	8.78
	BS-LL	6.12	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	8.8
Wong et al. (29)	BS-L-LS	4.58	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	8.79
(29)	BS-L-V2T10	4.73	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	10
	BS-L-V4T10	4.1	75.6	75.4	52	17.7	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	10.8
	BS-L-600	5.28	0	75.4	52	23.6	10.2	0.01	0.01	98.1	11.8	11.8	0.02	0.15	6.74
Ghobarah et	T1	4.48	61.7	61.6	65.8	15.8	9.84	0.01	0.01	108	15.7	9.84	0.02	0.19	12.1
al. (30)	T2	4.48	61.7	61.6	65.8	15.8	9.84	0.01	0.01	112	15.7	9.84	0.02	0.1	12.2
Karayannis et	<b>B</b> 0	4.59	84.3	84.3	39.4	11.8	7.87	0.01	0.01	59	11.8	7.87	0.01	0.05	8.18
al. (26)	C0	4.59	84.3	84.3	39.4	11.8	7.87	0.01	0.01	59	11.8	7.87	0.01	0.05	8.6
	L1	2.61	66.8	70.5	35.4	11.8	7.88	0.01	0.01	55.1	7.87	7.87	0.02	0.21	10.2
Tsonos et al. (31)	L2	2.61	66.8	70.5	35.4	11.8	7.88	0.01	0.01	55.1	7.87	7.87	0.02	0.21	11.6
(01)	01	2.61	66.8	70.5	35.4	11.8	7.88	0.01	0.01	55.1	7.87	7.87	0.02	0.21	10.2
Antonopoulos et al. (32)	C1	2.82	66.8	84.8	39.4	11.8	7.87	0.01	0.01	50.9	7.87	7.87	0.02	0.06	7.04
	C2	3.44	66.8	84.8	39.4	11.8	7.87	0.01	0.01	50.9	7.87	7.87	0.02	0.05	7.31
Sarsam et al. (33)	EX2	7.5	61.6	80	56	12	5.98	0.01	0.01	60	8.03	6.18	0.03	0.19	9.15

TABLE 1. Dataset Collection 1

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Filiatrault et al. (34)	<b>S</b> 1	4.93	69	69	78.8	17.7	13.8	0.01	0.01	118	13.8	13.7	0.03	0.08	12
Hoffschild et al. (35)	_	3.82	65.4	83.2	32.2	7.9	6.5	0.01	0.01	99.8	7.48	7.48	0.01	0.13	10.5
Park et al.	UJ2-EW	3.96	68.1	72.2	96	30	16	0.01	0.01	145	18	18	0.03	0.17	8.76
(36)	UJ2-NS	3.96	68.1	72.2	96	30	16	0.01	0.01	145	18	18	0.03	0.15	8.37
	UJ1-EW	4.3	70	68	96	18	16	0.02	0.02	145	18	18	0.03	0.31	14.4
	UJ1-NS	4.3	70	68	96	18	16	0.02	0.02	145	18	18	0.03	0.31	13.1
Hassan et al.	UJ2-EW	4.43	70	77	96	30	16	0.01	0.01	145	18	18	0.03	0.45	9.97
(37)	UJ2-NS	4.43	70	77	96	30	16	0.01	0.01	145	18	18	0.03	0.45	9.47
	BJ1-EW	4.41	70	77	96	18	16	0.02	0.02	145	18	18	0.03	0.45	11.4
	BJ1-NS	4.41	70	77	96	18	16	0.02	0.02	145	18	18	0.03	0.45	10.8
Salim et al. (27)	S1	4.39	68.1	66.8	35.8	11.8	5.91	0.02	0.01	74.8	7.09	7.09	0.02	0.09	8.59

The following factors are taken into consideration for the neural network's inputs in the current study: Joint width  $(b_j)$ , Joint depth  $(h_c)$ , Compressive strength of concrete  $(f_c)$ , Beam Reinforcement at the Top  $(T_{Ast})$ , Beam Reinforcement at the Bottom  $(B_{Ast})$ , Beam length (L), Yield strength of beam bars  $(f_{yb})$ , Joint Shear Reinforcement Index  $(\varphi_s)$ , Column Axial Load Level  $(P_y)$ , Beam Bar Index  $(x_b)$ , Beam-Column depth ratio

 $(h_b/h_c)$  and  $\tau$ . Table 2 displays the experiment analysis of the 53 data that were obtained for this investigation. The MATLAB scripting language is used to construct an object-oriented framework to collect certain joint specimen properties. A gathering of sample assets and measured outcomes, such as concrete strength, joint type, joint reinforcement ratio, etc., constitute an instance of the experiment class.

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S. no.	b <sub>j</sub>	h <sub>c</sub>	$f_c$	T <sub>Ast</sub>	B <sub>Ast</sub>	L	$f_{yb}$	$\varphi_s$	$P_y$	$x_b$	$h_b/h_c$	τ
1	280	300	31	0.806	0.806	1500	520	0	0	0.1538	1.5	3.75
2	280	300	33	0.806	0.806	1500	520	0.0819	0	0.1538	1.5	4.631
3	280	300	42	0.806	0.806	1500	520	0.1442	0	0.1538	1.5	5.7024
4	280	300	36	0.6045	0.6045	1500	520	0	0	0.1154	2	3.381
5	280	300	42	0.6045	0.6045	1500	520	0.0928	0	0.1154	2	4.2857
6	280	300	30	0.6045	0.6045	1500	520	0.2184	0	0.1154	2	4.0714
7	200	200	35	0.5234	0.5234	900	510	0.6602	0.1429	0.1333	1.5	4.3
8	200	200	35	0.5134	0.5134	900	495	1.0322	0.1429	0.0933	1.5	4.1
9	200	200	22	0.77	0.77	900	495	1.2184	0.2273	0.14	1.5	5.8
10	200	200	22	0.77	0.77	900	495	0.9767	0.2273	0.14	1.5	5.55
11	200	300	34	0.755	0.755	1000	580	0.2603	0.05	0.24	1	3.6333
12	200	300	34	0.755	0.755	1000	580	0.6764	0.05	0.24	1	3.45
13	200	300	32	0.785	0.785	1000	580	0	0.05	0.3	1	3.35
14	200	300	32	0.785	0.785	1000	580	0.0854	0.05	0.3	1	3.65
15	100	200	21	0.785	0.785	1000	470	0	0.1	0.2	1	3.3
16	100	200	21	0.785	0.785	1000	470	0.2564	0.1	0.2	1	3.6
17	100	200	21	0.785	0.785	1000	470	0.5179	0.1	0.2	1	3.6
18	100	200	23	1.18	1.18	1000	470	0	0.1	0.3	1	4.2

19	100	200	23	1.18	1.18	1000	470	0.245	0.1	0.3	1	4.85
20	100	200	23	1.18	1.18	1000	470	0.4949	0.1	0.3	1	4.4
21	200	200	36	0.2617	0.2617	1000	574	0	0.0486	0.0667	1.5	1.8
22	200	200	36	0.2617	0.2617	1000	574	1.0212	0.0486	0.0667	1.5	1.9
23	280	300	34	1.209	1.209	1500	520	0	0.1607	0.2308	1	6.0119
24	280	300	31	0.806	0.806	1500	520	0	0.1605	0.1538	1.5	3.75
25	280	300	36	0.6045	0.6045	1500	520	0	0.1607	0.1154	2	3.381
26	280	300	33	0.806	0.806	1500	520	0.1692	0.1605	0.1538	1.5	4.75
27	280	300	28	0.806	0.806	1500	520	0.3673	0.1607	0.1538	1.5	4.7976
28	280	300	33	0.806	0.806	1500	520	0.0819	0.1605	0.1538	1.5	4.631
29	280	300	42	0.806	0.806	1500	520	0.1442	0.1607	0.1538	1.5	5.7024
30	280	300	31	0.806	0.806	1500	520	0	0.1502	0.1538	1.5	3.7619
31	280	300	31	0.806	0.806	1500	520	0	0.1502	0.1538	1.5	4.0595
32	215	230	19	0.7137	0.7137	1375	300	0.2185	0.0798	0.2091	1.4348	2.8311
33	250	250	26	0.5491	0.5491	1375	300	0.7136	0.0615	0.1455	1.32	2.832
34	350	350	24	0.7272	0.7272	1780	417	1.5629	0	0.18	1.1429	3.4612
35	350	350	20	0.7272	0.7272	1780	417	1.7121	0	0.18	1.1429	3.6816
36	370	420	67	1.3639	1.3639	1900	430	1.0651	0.0188	0.2917	1.0714	6.4157
37	370	420	69	1.3639	1.3639	1900	430	1.3075	0.0183	0.2917	1.0714	7.2844
38	370	420	71	1.3639	1.3639	1900	430	1.1358	0.0178	0.2917	1.0714	6.9498
39	370	420	73	1.3639	1.3639	1900	430	1.1202	0.0173	0.2917	1.0714	6.686
40	200	200	16	0.77	0.77	1100	585	0	0.0719	0.14	1.5	2.925
41	200	200	19	0.77	0.77	1100	585	0	0.0605	0.14	1.5	2.875
42	200	200	15	0.77	0.77	1100	585	0.0839	0.0767	0.14	1.5	3.1
44	275	300	39	0.7856	0.7856	850	570	0	0	0.12	1.6667	2.3273
45	275	300	39	0.7856	0.7856	850	570	0	0.0932	0.12	1.6667	2.7152
46	275	300	37	0.7856	0.7856	850	570	0	0.1867	0.12	1.6667	3.3455
47	275	300	39	0.7856	0.7856	850	570	0	0	0.12	1.6667	2.9576
48	275	300	40	0.7856	0.7856	850	570	0	0.0909	0.12	1.6667	3.1515
49	275	300	38	0.7856	0.7856	850	570	0	0.1914	0.12	1.6667	3.6
50	275	300	43	0.7856	0.7856	850	485	0.2005	0	0.12	1.6667	4.1939
51	275	300	43	0.7856	0.7856	850	485	0.2005	0.0846	0.12	1.6667	4.6545
52	275	300	43	0.7856	0.7856	850	485	0.2005	0.1691	0.12	1.6667	4.7636
53	275	300	43	1.2872	1.2872	850	515	0.2005	0	0.1536	1.6667	4.4485

### **5. EXPERIMENTATION AND RESULTS DISCUSSION**

The suggested ANN model is created via MATLAB code and operates in MATLAB. The codes are developed in MATLAB with its toolbox. The dataset (input and output) used in this section is the same as the regression models' dataset. A popular training algorithm (so-called "Trainlm" (34)) that updates weight and bias values according to Levenberg-Marquardt optimization is used. Activation functions for the hidden and output layers are hyperbolic tangent sigmoid (Tansig) and linear transfer function (Purelin), respectively. To achieve the bestperforming model, a single ANN architecture is built with the hidden layer neurons set through experimentation (trial and error). Gradient descent is utilized to minimize error in the current study's backpropagation-type training procedure, which is used in shallow feed-forward with a single hidden layer. Using the Levenberg-Marquardt algorithm, the network is trained. The achievement of the ANN model is quantified using statistical metrics.

In Figure 4, the analysis focuses on the shear strength of beam-column joints according to various concrete grades. Specifically, this study employs grade M25 concrete and compares it with other grades such as M35, M40, and M30 across six different codes. The analysis aims to determine the shear strength of beam-column joints for each concrete grade within these codes. The results of this analysis reveal that the shear strength of M25 grade concrete in the beam-column joint is calculated as 2.6. This value indicates improved ductility and stiffness in the anchorage system, which can be attributed to reduced crack width and the formation of multiple cracks in the joint. Based on the findings, it can be concluded that the ACI 318-14 code provides a more suitable prediction for shear strength in the beam-column joint.

5. 1. Models Evaluation Measures To evaluate the constructed prediction models, a mathematical technique commonly employed in research to study machine learning models was utilized in this study. Several mathematical measures were employed to assess the accuracy of the models, including measures that aimed to minimize the discrepancy between the observed and predicted shear strength and others that aimed to identify the best-fit model. Eight evaluation measures were employed to accurately assess the anticipated accuracy of the models. These measures included the determination coefficient, Mean Square Error (MSE), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE). In evaluating the models, better performance is indicated by lower values of MSE and higher values of the determination coefficient ( $\mathbb{R}^2$ ), which should be closer to 1. By employing these evaluation measures, the study aimed to provide a comprehensive and accurate assessment of the predictive accuracy of the models.



Figure 4. Shear Strength of Joint with Several Codes

Figure 5 illustrates the Mean Squared Error (MSE) curve, which provides valuable insights into the training process. Initially, the error exhibits a rapid decline, indicating effective learning. As the training progresses, the rate of error reduction slows down. Notably, the MSEs of the validation data and test data follow a similar pattern to that of the training data, indicating the model's consistency and reliability. The minimum MSE value for the validation performance, reaching 0.00010534, is achieved after 13 training iterations. Importantly, no significant overfitting is observed up to this point, which is evident from the similar characteristics of the error in the test set and validation set. Consequently, the training results of this model can be considered reasonable and promising. The performance analysis for prediction accuracy is illustrated in Figure 6.

To evaluate the influence of different parameters on joint shear strength, a correlation coefficient is employed as defined in Equation 5. In this statistical approach, the



Figure 5. Mean Square Error Performance Analysis



Figure 6. Performance Analysis for Prediction Accuracy

independent variable x represents various parameters, while the dependent variable y represents the joint shear strength. Establishing a direct comparison between shear strength and each variable, this gain insights into their relationship. It is important to note that these correlation values provide approximate estimations of the parameters' impact on shear strength, as the correlations are expected to exhibit nonlinearity. While there may be correlations among the individual parameters, this analysis does not consider cross-correlations. The primary objective at this stage is to understand the degree of association between the parameters and joint shear strength.

Interestingly, the results indicate that the joint geometry has a relatively minor influence compared to the reinforcement ratio and axial load, which exhibit high correlation coefficients. This finding highlights the significance of the reinforcement ratio and axial load in determining joint shear strength.

The Levenberg-Marquardt method was used to train an optimised feed-forward neural network for each response parameter. Table 3 illustrates this neural network training and testing procedure with different initial, stooped, and target value parameters. To prevent overfitting, where the network perfectly matches the training data but performs poorly on the testing set, the number of epochs is kept to a minimum during the development of the optimal topology of the networks. Seven trained neural networks were used as experimental data and the findings of the FE study.

In Figure 7, the comparison between predicted and actual responses is displayed for different parameters of the response curves. The data points forming clusters along the diagonal line indicate the accuracy of the trained neural networks. The validation set was utilized to assess the generalizability of the model and to prevent overfitting by halting the training process. The R-squared ( $R^2$ ) value measures the proportion of variance in the response variable that can be predicted by the trained artificial neural network. In this study, the  $R^2$  values range from 0.92 to 0.99, indicating a high level of prediction accuracy. The ANN model achieves R-squared values of 99%, 94%, and 98% for the training,

**TABLE 3.** Testing and Training of Neural network model

Unit	Initial Value	Stopped Value	Target Value
Epoch	0	14	1000
Elapsed Time	-	00:00:00	-
Performance	22.8	0.0323	0
Gradient	65.6	0.0182	1e-07
Mu	0.001	0.001	1e+10
Validation Checks	0	6	6



**Figure 7.** Target Data versus Predicted Response in the Training, Validation, and Test Sets

testing, and validation sets, respectively, across all the data. These results demonstrate the robust performance of the ANN model in accurately predicting the responses, providing a reliable tool for estimating the desired parameters.

To ensure the superior robustness of the neural network model compared to traditional fitting methods, a random sampling method was employed for data set segmentation. Moreover, the Levenberg-Marquardt method was utilized for training the Self-Organizing Neural Network (SNN). The results, as presented in Table 4, highlight the overall superiority of ANN training and testing compared to other algorithms. This demonstrates that the proposed ANN model exhibits excellent alignment with experimental test results when compared to alternative models. Furthermore, the empirical model demonstrates improved performance compared to the results obtained from existing codes, emphasizing its effectiveness and accuracy.

**TABLE 4.** Results for Test Dataset with Existing Techniques

Test	ANN	STM	Emp
11.6	13.16	10.1	11.4
10.8	12.46	11.5	11
12.4	12.69	12.8	11.6
11.7	12.69	12.4	11.6
10.4	12.33	11.1	11
8.13	9.13	9.16	8.98
8.78	9.14	9.17	8.98
8.8	9.44	10.4	8.98
8.79	9.15	9.25	8.98

10	9.19	9.37	8.98
10.8	9.04	8.83	8.98
6.74	8.55	8.11	7.78
12.1	11.44	12	11.3
12.2	11.32	10.7	11
8.18	7.83	9.79	11
8.6	7.83	9.62	11
10.2	10.20	7.99	9.21
11.6	10.20	7.79	9.21
10.2	10.20	7.79	9.21
7.04	7.13	6.79	8.98
7.31	7.36	7.27	8.98
9.15	10.72	11.9	9.15
12	9.88	10.4	9.7
10.5	8.96	10.8	10.7
8.76	7.77	8.81	8.57
8.37	7.66	8.79	8.52
14.4	11.82	13.2	12
13.1	11.82	13.2	12
9.97	9.48	10.2	9.55
9.47	9.48	10.4	9.55
11.4	11.66	10.1	9.06
10.8	11.66	10.2	9.06
8.59	9.31	9.34	8.52

In Figure 8, several plots depict the analysis of the full data set, including the correlation coefficient (CC) plot comparing actual values with predicted values, the error histogram, and the graph illustrating predicted versus accurate shear strength values. Figure 8a presents the CC plot, where a correlation coefficient of 98.24% demonstrates a strong correlation between the predicted values and the actual values. This indicates that the ANN model's predictions align well with the true values. Figure 8b displays an error histogram, showcasing the distribution of errors between the predicted and actual



Figure 8. CC Plot for Actual and Predicted Values

shear strength values. Approximately 85% of the predictions made by the ANN model fall within a 9% margin of error. This suggests that the model performs well in accurately estimating the shear strength values, with a relatively small margin of error for the majority of predictions. These visualizations highlight the effectiveness of the ANN model in capturing the correlation between predicted and actual shear strength values and demonstrate its ability to generate accurate predictions for the full data set.

In Figure 9, a performance analysis graph is presented, comparing precision and recall for concrete cracking, spalling, rebar exposure, and rebar buckling. The objective was to evaluate the network's performance as the percentage of modules varied and to analyse its impact on the model's effectiveness. The curve precision-recall (PR) was employed for this assessment, as shown in Figure 9.

For the cracking model, the obtained values range from 0.764 to 0.831. Notably, the proposed SFF-ANN network achieves an accuracy that is 8.8% higher compared to other models, indicating its improved performance in predicting concrete cracking. The PR curve provides insights into the precision and recall achieved by the model, offering a comprehensive evaluation of its performance across different scenarios. The results demonstrate the superiority of the SFF-ANN network in accurately predicting concrete cracking, leading to enhanced accuracy and improved performance compared to alternative models.

In Figure 10, a comparison analysis is presented, comparing the performance of the Artificial Neural



Figure 9. Precision Vs Recall Performance Graph



Figure 10. Comparison Analysis of ANN with Two Datasets

Network (ANN) with the Strut and Tie Model (STM) and Empirical Model (Emp). Figure 10(a) focuses on the analysis of the ANN test data using dataset 1. The plot showcases the regression lines for the three models, representing the line of best fit that minimizes the total error of the model. It is important for the relationship between variables to be linear, and this can be visually assessed through a scatter plot. In this case, the data points exhibit a distribution implying a linear relationship. In Figure 10(b), a comparative analysis is conducted using dataset 2, and the regression plot is determined for the ANN, ACI, and Eurocode models. The scatter plot in this case does not align in a straight line but appears more scattered. This indicates that in the comparative study of ANN, the collected dataset performs better when compared to dataset 2. These visualizations in Figure 10 provide insights into the comparative performance of the ANN model against the Strut and Tie Model (STM) and Empirical Model (Emp.). The results suggest that the ANN model shows promising performance, particularly when compared to the specific datasets analyzed in this study.

## **6. RESEARCH CONCLUSION**

The article successfully developed an artificial neural network (ANN) model using artificial intelligence technology to assess the reinforced concrete shear ability of external beam-column (BC) joints. Experimental data from various literature works were gathered and assembled to create an input and output data set for the ANN model. The proposed ANN model outperformed other models and empirical formulas provided in design codes in terms of precision and accuracy.

- The ANN-based model, implemented in MATLAB, can effectively predict the shear strength of external BC joints made of reinforced concrete.
- Five main parameters, namely joint aspect ratio, joint transverse reinforcement, concrete compressive strength, beam reinforcement ratio, and joint width, were used to develop the ANN model.
- The ANN model's effectiveness was quantitatively assessed using the coefficient of determination (R<sup>2</sup>), with R-squared values of 99%, 94%, and 98% obtained during the training, testing, and validation stages, respectively.
- Comparison of the ANN model results with experimental data showed strong agreement and better alignment compared to results calculated using various design codes such as ACI 318-14, EN 1998-1:2004, NZS 3101-1:2006, CSA A3.3:2004, AIJ:2010, and IS 13920:2016.
- The proposed SFF-ANN model, which combines the ANN model with experimental data, is considered an efficient tool for predicting the shear strength of interior joints exposed to cyclic loading.

In conclusion, this research contributes to the scientific field by introducing an ANN model that outperforms existing empirical formulas and design codes in accurately predicting the shear strength of reinforced concrete external BC joints. The study's findings have significant practical implications, as the developed model can be applied to real-world projects, providing engineers with a reliable tool for assessing the performance and structural integrity of external BC joints. This joint shear strength prediction model can be readily implemented into joint response models for the evaluation of earthquake performance and inelastic responses of building frames.

Consequently, the proposed model holds tremendous potential as a valuable resource for researchers and reinforced concrete engineers, enabling them to make precise estimations of the joint shear strength of beamcolumn connections. This model proves particularly advantageous in two key aspects: it operates within the input data ranges established in this study, ensuring accuracy, and it significantly reduces both time and cost compared to the construction of alternative numerical schemes. As such, this model emerges as an efficient and cost-effective tool for professionals in the field, streamlining the estimation process while maintaining reliability. Further research should focus on gathering field data and conducting comparative studies to validate the model's predictions and explore its applicability in diverse structural configurations.

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*چکید*ه

#### Persian Abstract

شکست اتصالات تیر و ستون نوع برشی در قاب های بتن مسلح (RC) در هنگام حملات شدید زلزله یک نگرانی حیاتی است. روش های ستی برای تعیین ظرفیت برشی اتصال اغلب به دلیل در نظر گرفتن نادرست پارامترهای حاکم بر رفتار این اتصالات، دقت کافی ندارند. این مطالعه قابلیت های تکنیک های یادگیری ماشین را در پیش بینی ظرفیت برشی مشترک و حالت های شکست برای اتصالات تیر ستون خارجی، با توجه به رفتار ساختاری پیچیده آناه ارزیابی میکند. یک مدل شبکه عصبی مصنوعی (ANN) برای پیش بینی مقاومت برشی اتصالات تیر ستون خارجی تقویت شده پیشنهاد شده است ANN ، جزء هوش مصنوعی که از تجربیات گذشته درس می گیرد، در مهندسی عمران معروبیت پیدا می کند. مدل ANN با استفاده از مجموعه داده ای شامل خواص مواد، ابعاد نمونه و شرایط بارگذاری لرزه ای از تحقیقات تجربی قبلی توسعه یافته است. این مدل دوازده پارامتر ورودی را برای پیش بینی مقاومت برشی در اتصالات تیر ستون خارجی در نظر می گیرد. آموزش و آزمایش مدل ANN با استفاده از کدهای طراحی ایجاد مدل دوازده پارامتر ورودی را برای پیش بینی مقاومت برشی در اتصالات تیر ستون خارجی در نظر می گیرد. آموزش و آزمایش مدل ANN با استفاده از کدهای طراحی ایجاد شده، فرمول های تجربی و یک الگوریتم خاص انجام می شود. نتایج نشاندهنده بر تری شبکه عصبی مصنوعی پیشروی کم عمق (ANN با ستفاده از کدهای طراحی ایجاد شده، فرمول های تجربی و یک الگوریتم خاص انجام می شود. نتایج نشاندهنده بر تری شبکه عصبی مصنوعی پیشروی کم عمق (ANN با ستفاده از کدهای طراحی ایجاد شده، فرمول های تجربی و یک الگوریتم خاص انجام می شود. نتایج نشاندهنده بر تری شبکه عصبی مصنوعی پیشروی کم عمق (ANN با ستفاده از دمقایسه با رویکردهای شرمون از را بنشی یک مدل شبکه عصبی مصنوعی(ANN) به صورت کمی در این مطالعه با تمرکز بر عملکرد آن در مقایسه با کدهای طراحی مختلف که معمولاً در مهندسی سازه استفاده می شوند، ارزیابی شد. مدل با استفاده از ضریب ۹۹٪ می بر ای اتصالات تیر سوی به در طول مراحل آموزش، آزمایش و این استه از را بینی مطالعه اهمیت تقویت تیر را به عنوان یک عنصر کلیدی در برآورد ظرفیت برشی برای اتصالات تیر سون SPS جارجی بر جسته می کند. اگرچه مدل این این می دریه بالی می مدل با استفاده از ضریب تعیین (R) این می و مقادیر R-squad به برای این تیرمون SPS بارجی مرحی و مدی می می بر وی مول می و می می می و میرای می م



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# Predictive Modelling and Optimization of Double Ring Electrode Based Cold Plasma Using Artificial Neural Network

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#### **1. INTRODUCTION**

Plasma is considered the fourth state of matter and is considered as ionized gas (1). Plasma is generated due to the association of strong electromagnetic field, gas and heat. Generally, reactive nitrogen and oxygen species (RONS) (2) have a main role in atmospheric pressure plasma formation (APP). As the key components of air are oxygen and nitrogen, reactive oxygen species (ROS) comprise of hydroxide and oxygen radicals, while nitrogen oxides are included as reactive nitrogen species (RNS) (3). The APP generates neutral reactive species, free electron, atom such as oxygen (O) and molecules, radicals and nitrogen oxide (NO) (4-6). Cold atmospheric pressure plasma (CAP) is applications in many fields such as: sterilization (6), surface modification (7), food safety (8), water purification (9), textiles (10), medical (11) and others. The effect of CAP is very unique and it is for specific application.

Amongst the various technologies implemented for generating atmospheric cold plasma, there are two major

ABSTRACT

Cold Atmospheric Pressure Plasma (CAP) is very potent and impactful technology implemented for both technological and biomedical applications. This paper focuses on the implementation of artificial neural network (ANN) for a novel double ring electrode based cold atmospheric pressure plasma which is to operated only in the glow discharge region for its application in biomedical field. ANN inherently helps in visualizing the effective output parameters such as peak discharge current, power consumed, jet length (with sleeve) and jet length (without sleeve) for given set of input parameters of supply voltage and supply frequency using machine learning model. The capability of the ANN model is demonstrated by predicting the output parameters of the CAP beyond the experimental range. Finally, the optimized settings of supply voltage and supply frequency will be determined using the composite desirability function approach to simultaneously maximize the peak discharge current, jet length (with sleeve), and minimize the power consumption.

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categories which are dominant in clinical and preclinical research in the field of plasma medicine which includes plasma jets (12-15) and dielectric barrier discharge (DBD) (16, 17). In DBD's the plasma is ignited in the gap between the powered and ground electrode. There are various types of DBD's such as volume DBD, Surface DBD used for various applications. The plasma jet experimental typically comprises of tube-like structure such as quartz tube, the plasma is generated using a working gas such as argon that would flow inside this tube. There are various electrode designs such as DBDlike jets, DBD jets and single electrode jets. The gas flow inside the quartz tube enables the resulting plasma to be carried out and is focused on the target material to be treated. Mostly noble gases are used as working gases for the generation of plasma jet.

ANN has been applied successfully in plasma medicine; Lin et al. (18) implemented ANN approach for predicting gas compositions and gas temperature using spontaneous emission spectroscopy, wherein the ANN output is used to control the power consumption of the

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device and gas injection rate, thereby optimizing the plasma chemistry. Furthermore, Wan et al. (19) implemented an ANN model to predict NO conversion by DBD in the N<sub>2</sub>/O<sub>2</sub>/NO system. Their ANN model results indicated that the primary factor influencing the production of NO<sub>2</sub> is the concentration of NO at the inlet, responsible for 36.22% of the effect. The other factors that impacted NO<sub>2</sub> production were discharge power at 23.52% and residence time at 26.25%.

The cold plasma technology involves various important operating parameters, viz., supply voltage (SV), supply frequency (SF), pulse discharge current (PDC), jet length and power consumption (P) (11). From the perspective of development of CAP devices, it is of vital importance to determine the optimum levels of input parameters of supply voltage and supply frequency to achieve the desired levels of pulse discharge current, jet length and power consumption. Furthermore, since experimental tests usually have certain limitations with respect to the range of parameters, an accurate and reliable predictive model can be useful to make performance predictions beyond the range of parameters considered in the experiments. Recently, one of the robust and popular machine learning techniques called artificial neural network (ANN) has been implemented to predict the efficiency of CAP-based technologies in terms of the input parameters towards applications such as plasma treatment and CO<sub>2</sub> splitting (20, 21). However, there is a paucity of research in the literature on development of predictive models for the fundamental performance characteristics such as PDC, jet length and power consumption. This paper aims to develop an ANN model for the novel double ring electrode based cold atmospheric pressure plasma using a benchmark experimental data (11) to train, test and validate the model. The robustness of the neural network to model the physics of the cold plasma device is demonstrated by making performance predictions beyond the range of the experimental data used for training the model. Finally, the well-established statistical method of desirability function analysis (DFA) will be used to perform the multi-response optimization to determine the optimum settings of the input parameters for the best performance.

#### 2. GEOMETRY AND EXPERIMENTAL SETUP

The double ring electrode configuration (11)examined in this paper comprises of quartz tube with nozzle as shown in Figure 1. Ring electrodes are the two metal sleeves that are put on top the nozzle indicated as 3 in Figure 1. One of these electrodes is connected to supply and another electrode is grounded. The nozzle outlet diameter is 3 mm and has been indicated as 2 (see Figure 1). The working gas used Argon enters through the inlet of quartz tube indicated as 1 (see Figure 1). The outer diameter and length of quartz tube is 25 mm and 155 mm, respectively. The quartz tube thickness is 1.5 mm. The diameter and axial length of ring electrodes are 4 mm and 18 mm respectively. The ring electrodes are separated by distance of 3 mm as indicated -3 in Figure 1. A quartz sleeve of 4 mm diameter and 15 mm length was placed on the nozzle of the quartz tube (see Figure 2) to observe the length of plasma jet without the effect of surrounding air. To examine the plasma jet length without the effect of surrounding air, a quartz sleeve of 15 mm length and 4 mm diameter was placed on nozzle of quartz tube (Figure 2). Jet length was examined for both without and with quartz sleeve.

The double ring electrode implemented in this paper has been subjected to supply voltages upto 6 kV and supply frequencies upto 25 kHz. Working gas employed was Argon as shown in Figure 2. The V-I characteristic of the developed DBD-based cold plasma jet (Figure 2) has been studied and the consumption of power has been analyzed at various input combinations (supply voltage and frequency). The supply frequency and voltage have been varied from 10 to 25 kHz and 3.5 to 6 kV, respectively. The gas flow rate is fixed at 1 liter/min. The experimental results of pulse discharge current (PDC), jet length without and with sleeve (JLwoS and JLwS) and power (P), for the various supply voltage and supply frequencies is listed in Table 1.

In this paper, ANN is implemented for the experimental data as listed in Table 1 to analyze and



Figure 1. Geometry of double ring electrode based cold plasma jet using Argon



Figure 2. Argon based cold plasma jet using double ring electrode

	IAD	LE I. EX	Jermen	allesuits	[11]	
Expt. No.	SV (kV)	SF (kHz)	PDC (mA)	JLwoS (mm)	JLwS (mm)	P (W)
1	3.5	10	152	2	5	0.28
2	4	10	160	4	7	0.33
3	4.5	10	176	7	9	0.46
4	5	10	144	12	15	0.46.
5	5.5	10	176	15	21	0.56
6	6	10	192	17	22	0.42
7	3.5	15	96	4	7	0.33
8	4	15	112	6	9	0.58
9	4.5	15	152	8	12	0.58
10	5	15	144	14	17	0.69
11	5.5	15	176	18	23	0.78
12	6	15	232	20	24	0.63
13	3.5	20	88	6	10	0.59
14	4	20	128	8	12	0.73
15	4.5	20	112	12	15	0.82
16	5	20	152	18	22	1.12
17	5.5	20	168	20	25	1.04
18	6	20	184	22	27	0.72
19	3.5	25	88	8	12	0.94
20	4	25	96	11	14	0.89
21	4.5	25	152	12	17	0.88
22	5	25	128	22	25	0.97
23	5.5	25	144	24	28	1.27
24	6	25	216	25	29	1.04

predict the output parameters (discharge current, jet length (with and without sleeve) and power consumption for higher values of supply voltage and supply current for the double ring electrode-based argon cold plasma jet.

## **3. ANN APPROACH**

Artificial neural network (ANN) is a soft computing paradigm which derives its functionality through inspiration from the neurons in the biological nervous systems. ANN operates with a similar principle of that of biological neurons wherein the information processing takes place in the individual neurons starting with a feedforward training process, also involving a backpropagation feedback loop to estimate the errors in prediction, to derive a mathematical formulation to model the relationship between process parameters and the output responses (22).



**Figure 3.** General architecture of a single hidden layer NN model with *n* neurons

In the simplest configuration, a neural network model consists of an input layer which consists of the input parameters, followed by a hidden layer which consists of an arbitrary number of neurons according to the requirements of the problem, and finally the output layer which is nothing but the list of the output parameters (Figure 3). In this study, a multi-layer perceptron ANN model was developed using the *fitnet* function in MATLAB (MathWorks, Natick, Massachusetts, USA). The multi-layer perception basically falls into the category of neural networks with more than one hidden layer. To ensure a good predictive accuracy of the model, the possibility of having one or more hidden layers was investigated. The Levenberg-Marquardt algorithm was employed for training the model (23). The inputs are the two control parameters, i.e., SV and SF; and the outputs are the four response parameters, PDC, JLwS, JLwoS, and P.

The input data was divided into three sets such that 70% of it was used for training and remaining 15% each were used for testing and validation of the network. Numerous trials were conducted with the number of hidden layers and the number of neurons in them to arrive at a model which provided a good descriptive performance (refer Appendix for details), which is then made use to make predictions beyond the experimental range of control parameters.

Each neuron in the artificial neural network consists of three components, weights  $(w_{k,j})$ , biases  $(b_k)$ , and an activation function. The weights and biases are fed to individual neurons along with the inputs to obtain the mathematical operation in each neuron as Equation (1) (24):

$$U_{k} = b_{k} + \sum_{j=1}^{n} w_{k,j} \times I_{j}$$
(1)

where, n is the number of inputs and k signifies the  $k^{th}$  neurons in the hidden layer. The same equation can be written in the matrix form as Equation 2 (22):

$$U_{k} = \begin{pmatrix} w_{11} & \dots & w_{1n} \\ \vdots & \ddots & \vdots \\ w_{m1} & \dots & w_{mn} \end{pmatrix}_{m \times n} \begin{bmatrix} I_{1} \\ \vdots \\ I_{n} \end{bmatrix}_{n \times 1} + \begin{bmatrix} b_{1} \\ \vdots \\ b_{n} \end{bmatrix}_{m \times 1} = \begin{bmatrix} U_{1} \\ \vdots \\ U_{n} \end{bmatrix}_{m \times 1}$$
(2)

The inputs and outputs in each neural network are typically normalized between [-1, +1]. Finally, the overall mathematical relationship to predict the output 'Y' can be written as Equation 3 (22):

$$Y = b_{output-layer} + \sum_{k=1}^{m} LW_k \times f(U_k)$$
(3)

where,  $b_{output-layer}$  is the output layer weight and  $LW_k$  is the layer weight matrix. The activation function f(x) is a tan-sigmoid (*tansig*) or hyperbolic tangent function as shown by Equation 4 (23):

$$f(U_k) = \frac{2}{1 - e^{-2U_k}} - 1$$
(4)

In this study, the *tansig* function was used for the connections between the input and hidden layers and the hidden layers to output layers [20-22]. The descriptive accuracy of the model was evaluated based on the coefficient of determination ( $R^2$ ), which is given by Nateghi- and Ahmadi (24):

$$R^{2} = 1 - \frac{\sum_{i} (y_{i} - y_{exp-i})^{2}}{\sum_{i}^{n} (y_{i} - \overline{y}_{exp-i})^{2}}$$
(5)

where,  $y_i$  and  $y_{exp-i}$  are the model predictions and the corresponding experimental data, respectively, and  $\bar{y}_{exp-i}$  indicates the mean of the experimental response, for a particular response parameter.

## 4. DESIRABILITY FUNCTION ANALYSIS

n

Desirability Function Analysis (DFA) is a statistical method used for multi-response optimization, particularly in the field of experimental design and quality improvement. It provides a way to simultaneously optimize multiple responses or variables in a process or system. The main idea behind DFA is to convert individual response variables into a single overall desirability value.

Firstly, the individual desirability function for each factor setting is calculated. This is called as the desirability index (DI). Next, the overall desirability for a particular combination of factor settings, termed as composite desirability index (CDI), is calculated as the geometric mean of the individual desirability values. This approach ensures that all responses contribute equally to the overall desirability assessment [25-27].

$$d_{i} = \begin{cases} 0 & y_{i} < y_{\min} \\ \left(\frac{y_{i} - y_{\max}}{y_{\max} - y_{\min}}\right)^{s} & y_{\min} \le y_{i} \le y_{\max}, s \ge 0 \\ 1 & y_{i} > y_{\max} \end{cases}$$
(6)

$$d_{i} = \begin{cases} 1 & y_{i} < y_{\min} \\ \frac{y_{i} - y_{\max}}{y_{\min} - y_{\max}} \\ 0 & y_{i} > y_{\max} \end{cases}^{r} y_{\min} \leq y_{i} \leq y_{\max}, r \geq 0$$
(7)

The goal of DFA is to find the factor settings that maximize the overall desirability (or CDI). This can be achieved using optimization techniques such as response surface methodology. By optimizing the overall desirability, DFA helps identify the factor settings that simultaneously optimize multiple responses and improve the quality or performance of a process or system.

The principle of DFA first propounded by Harrington in 1965 (25) was refined and brought to its presently used form by Derringer and Suich in 1980 (26). The method of DFA is enunciated as follows. Firstly, based on the criteria of whether a response variable needs to be maximized (larger-the-better) or minimized (smaller-the-better), the desirability index (DI) for each factor setting combination is calculated using the Equations 6 and 7, respectively (27).

Equations 6 and 7,  $y_{min}$  and  $y_{max}$  indicate the minimum and maximum of the response  $y_i$ . The exponents *s* and *r* are the weights assigned to each response variable. Here, we assign equal weightage to all the response, implying, s = r = 0.25. In this study, the PDC and P were subjected to the condition of smaller-the-better, whereas the larger-the-better condition was imposed on JLwS and JLwoS. Now, the composite desirability index (CDI) is computed as follows (27):

$$CDI_{i} = \left(d_{i,1}^{w_{1}} \times d_{i,2}^{w_{2}} \times d_{i,3}^{w_{3}} \times \dots \times d_{i,k}^{w_{k}}\right)^{1/k}$$
(8)

where, k indicates the number of responses (here, k = 4),  $d_{i,k}^{w_k}$  represents the desirability index of the  $k^{th}$  response and  $w_1$ ,  $w_2$ ,  $w_3$ ,..., are the weightages assigned to individual responses, such that  $\sum_i^k w_i = 1$ . Here, we assign equal weightage, implying,  $w_i = 0.25$ . Now, the mean of factor effect at each level is analyzed to obtain the best combination of the control parameters to achieve the maximum possible CDI (27). The maximum possible CDI signifies the optimized control parameter setting combination at which the multiple responses are achieving their best possible combinatorial outcome.

## **5. RESULTS AND DISCUSSION**

**5. 1. Descriptive and Predictive Modeling using Artificial Neural Network** The artificial neural network for modeling the performance of the double ring electrode based cold plasma jet was developed by a trialand-error approach by varying the number of hidden layers and the number of neurons in them. The number of layers were varied from 1 to 3, and in each layer, the number of neurons were changed from 3 to 20. During these trials, the descriptive accuracy of the model was evaluated by means of the coefficient of determination ( $R^2$ ) for each of the four performance parameters (PDC, JLwS, JLwoS and P). It was found that, a two-layered ANN with 8 and 12 neurons, in the first and second hidden layers, respectively (Figure 4), provided the best descriptive accuracy with  $R^2 > 0.96$  for all the parameters. Figure 5 graphically depicts the descriptive accuracy of the ANN model for the parameters. Table 2 (Expt. No. 1 – 24) lists the numerical predictions of the ANN model for the experimental data shown in Table 1.

A robust model not only needs to accurately model the experimental data, but also make predictions for new set of data beyond the experimental range, while being consistent with the physics of the problem. After confirming the descriptive accuracy of the ANN model, its predictive capability is investigated by forecasting the performance parameters beyond the range of control parameters used in the experiments. Table 2 (Expt. No.25 – 56) shows the predictions of the ANN model for 6.5 kV  $\leq$  SV  $\leq$  10 kV and 10 kHz  $\leq$  SF  $\leq$  25 kHz.

The split of the datasets for training, testing and validation steps were chosen randomly in each trial using the MATLAB function dividerand, which splits the data based on random indices. For the optimum model (2-8-20-4) the expt no. 1, 3, 5, 7, 8, 9, 10, 11, 12, 13, 14, 15, 17, 18, 20, 21, 23 were used for training, expt no. 16, 29, 22, 24 were used for validation and remaining (2, 4, 6, 19) were used for testing purposes.

From Table 2, for (3 kV, 10 kHz) the power consumed in the plasma is 0.33 W with short plasma jet lengths (5.1 mm (JLwS), 2.1 mm (JLwoS)), as the energy is consumed by the seed electrons for plasma generation. Whereas, when supply voltage approaches 6 kV, 10 kHz then power consumption is 0.56 W with longer jet lengths (26.1 mm (JLwS), 20.3 mm (JLwoS)) indicating that power is utilized for plasma generation. It is also observed that plasma jet lengths with sleeve for most cases of supply voltages and frequency (3.5 kV – 10 kV,



Figure 4. ANN architecture with '2-8-20-4' topology



**Figure 5.** Comparison of ANN predictions for (a) PDC, (b) JLwS, (c) JLwoS, (d) P, with the corresponding experimental responses

Expt. No.	SV (kV)	SF (kHz)	PDC (mA)	JLwoS (mm)	JLwS (mm)	P (W)
1	3.5	10	152.0	5.1	2.1	0.33
2	4	10	165.9	5.4	2.4	0.38
3	4.5	10	176.0	9.0	7.0	0.46
4	5	10	134.4	15.7	13.6	0.53
5	5.5	10	176.0	21.0	15.0	0.55
6	6	10	229.1	26.1	20.3	0.56
7	3.5	15	96.0	7.0	4.0	0.39
8	4	15	112.0	9.0	6.0	0.52
9	4.5	15	152.0	12.0	8.0	0.62
10	5	15	144.0	17.0	14.0	0.70
11	5.5	15	176.0	23.0	18.0	0.77
12	6	15	231.9	24.0	20.0	0.63
13	3.5	20	88.1	10.0	6.0	0.59
14	4	20	128.0	12.0	8.0	0.70
15	4.5	20	112.0	15.0	12.0	0.85
16	5	20	152.0	22.0	18.0	1.07
17	5.5	20	168.0	25.0	20.0	1.03
18	6	20	184.0	27.0	22.0	0.74
19	3.5	25	89.1	10.7	9.1	0.82
20	4	25	96.0	14.0	11.0	0.88
21	4.5	25	152.0	17.0	12.0	0.87
22	5	25	128.0	25.0	22.0	1.04
23	5.5	25	144.0	28.0	24.0	1.18
24	6	25	216.0	28.9	24.9	1.06
25	6.5	10	232.0	26.6	22.5	0.53
26	7	10	232.0	26.1	23.2	0.52
27	7.5	10	232.0	25.7	23.5	0.51
28	8	10	232.0	25.5	23.6	0.50
29	8.5	10	232.0	25.4	23.6	0.50
30	9	10	232.0	25.4	23.6	0.50
31	9.5	10	232.0	25.4	23.6	0.50
32	10	10	232.0	25.4	23.6	0.50
33	6.5	15	232.0	25.6	22.9	0.54
34	7	15	232.0	25.8	23.4	0.52
35	7.5	15	232.0	25.7	23.5	0.51
36	8	15	232.0	25.6	23.6	0.51
37	8.5	15	232.0	25.5	23.6	0.50
38	9	15	232.0	25.5	23.6	0.50
39	9.5	15	232.0	25.4	23.6	0.50

TABLE	2.	ANN	predictions	for	within	the	range	of
experime	ntal	data pr	ovided in Tał	ole 1	and beyo	ond th	ne range	e of
supply vo	ltag	e (6 kV	$f \le SV \le 10 \text{ k}^3$	V and	110 kHz	$\leq$ SF	$\leq 25 \text{ kl}$	Hz)

40	10	15	232.0	25.4	23.6	0.50
41	6.5	20	220.0	27.7	23.5	0.56
42	7	20	229.2	27.5	23.6	0.52
43	7.5	20	231.5	27.1	23.4	0.51
44	8	20	231.9	26.8	23.3	0.51
45	8.5	20	232.0	26.5	23.3	0.51
46	9	20	232.0	26.2	23.4	0.51
47	9.5	20	232.0	26.0	23.5	0.51
48	10	20	232.0	25.9	23.5	0.51
49	6.5	25	223.7	29.0	25.0	0.85
50	7	25	222.9	29.0	25.0	0.74
51	7.5	25	220.7	28.9	24.9	0.67
52	8	25	217.8	28.9	24.9	0.62
53	8.5	25	216.2	28.8	24.7	0.58
54	9	25	218.1	28.6	24.5	0.55
55	9.5	25	223.4	28.3	24.2	0.53
56	10	25	228.6	27.8	23.8	0.52

10 kHz – 25 kHz) is longer as compared to jet length without sleeve as seen in Table 2. This is because the sleeve shields the plasma jet coming out from electronegative gases such as water vapor that impede the propagation of the plasma jet. The power consumed by the plasma jet increases as the supply voltage and frequency reaches up to 6 kV, 25 kHz (1.06 W). Any higher supply voltage resulted in the power being lost in heating of dielectric tube and not utilized in the plasma generation which is clearly seen in Table 2 indicating the decrease in power consumed (0.85 W at 6.5 kV, 25 kHz).

It can be further seen from Table 2 that at higher voltages of (6.5 kV, 10 kHz – 25 kHz) there is only variation of power consumption (0.53 W – 0.85 W) by the plasma as most of the power supplied is not utilized in the plasma generation but lost in the dielectric material as thermal dissipation, leading to heating of the dielectric tube. However, at (6.5 kV, 10 kHz – 25 kHz) the plasma jet length both with and without sleeve increases (26.6 mm – 29 mm (JLwS), 22.5 mm – 25 mm (JLwoS)) with increase in supply frequency. This is due to the higher energy absorbed by the seed electrons at higher supply frequency (20 kHz – 25 kHz) resulting in longer jet lengths as seen in Table 2.

A similar result has been observed at (7.5 kV, 10 kHz – 25 kHz) where there is only slight variation in the power consumed (0.51 W – 0.67 W) due to supply power being lost in thermal dissipation of the material. Further higher voltages of 8.5 kV - 10 kV (10 kHz – 25 kHz) also show only a slight variation in the power consumption as the supply power is lost as thermal dissipation. However, at (7.5 kV, 10 kHz – 25 kHz) the plasma jet length both

with and without sleeve increases (25.7 mm – 28.5 mm (JLwS), 22.5 mm – 25 mm (JLwoS)) with increase in supply frequency. This is due to the higher energy absorbed by the seed electrons at higher supply frequencies (20 kHz – 25 kHz) resulting in longer jet lengths as seen in Table 2.

But at supply voltage of (8.5 kV - 10 kV, 25 kHz)there is hardly any variation of power consumed as seen in Table 2; in fact, the power consumed reduces from 0.58 W (8.5 kV/25 kHz) to 0.52 W (10 kV/25 kHz) due to power supply lost in thermal dissipation of dielectric material and also as the plasma discharge approaches the arc discharge region which is not suitable for biomedical applications. Due to this thermal dissipation heat loss at (8.5 kV - 10 kV, 25 kHz) it must be observed that there is a decrease in plasma jet length (28.8 mm - 27.8 mm (JLwS), 24.7 mm - 23.8 mm (JLwoS)) which is evidently indicating that the power supply is not being utilized in the generation of plasma.

5. 2. Multi-Response Optimization using DFA and **Optimum Level Prediction using ANN** For the multi-response optimization, firstly, the desirability indices  $(d_i)$  are calculated using Equations 6 and 7. The parameters JLwS and JLwoS were maximized using Equation 6, whereas PDC and P were minimized using Equation 7. Table 3 shows the  $d_i$  of the four response parameters (PDC, JLwS, JLwoS and P) for each experimental trial shown in Table 2 under the column of individual desirability  $(d_i)$ . Subsequently, the composite desirability indices (CDI) are calculated to take simultaneously optimize the multiple response parameters (Table 3). Finally, the values of CDI are ranked in the descending order from highest to the lowest value to determine the best possible combination of the control parameter to achieve the best performance of the double ring electrode based cold plasma jet. It is observed that, Expt. No. 22 with SV = 5 kV and SF = 25 kHzprovides the best performance (highlighted in boldface in Table 3).

To statistically evaluate the factor effects on CDI, its main effect plot is shown in Figure 6(a). It is found that the mean of means of CDI becomes maximum for the control parameter setting of SV = 5 kV and SF = 25 kHz, which is consistent with the results of DFA. Further, a contour plot of CDI is presented in Figure 6(b), wherein its variation is better visualized with respect to the interaction of SV and SF. Here, it is observed that SV < 6 kV results in CDI > 0.6 for almost the entire range of SF. However, for SV > 6 kV, the SF needs to be > 23 kHz to obtain a higher performance output. Also, it can be ascertained that SV = 5 kV and SF = 25 kHz yields the best output since it achieves the maximum CDI (> 0.8).

Regarding the fact that plasma processes require several factors, each of which may have a substantial effect on plasma production. An artificial neural network (ANN) can be used to analyze and predict the impact of such elements with different values operational parameters (supply voltage & supply frequency). For instance, in our study the pulsed power supply cannot be operated at higher voltages such as 7 kV- 10 kV due to physical constraints of the device. Hence, ANN served to be a potent predictive tool for estimating the performance of the device with higher level of accuracy at those operational range (7-10 kV). Also, ANN is highly impactful in analyzing the sensitivity of each of input variables with the performance output such as power consumption, jet length (with/without sleeve).

**TABLE 3.** Estimated desirability indices using DFA

Expt.	Ind	ividual de	CDI	<b>D</b> 1		
No.	PDC	JLwoS	JLwS	Р	CDI	капк
1	0.8633	0.0000	0.0000	1.0000	0.0000	46
2	0.8409	0.5373	0.5430	0.9871	0.7015	31
3	0.7897	0.6389	0.6828	0.9511	0.7566	29
4	0.8842	0.8034	0.8120	0.9511	0.8606	7
5	0.7897	0.9036	0.8671	0.9202	0.8687	4
6	0.7260	0.9174	0.8987	0.9626	0.8712	3
7	0.9858	0.5373	0.5430	0.9871	0.7300	30
8	0.9554	0.6389	0.6458	0.9137	0.7747	26
9	0.8633	0.7349	0.7147	0.9137	0.8023	21
10	0.8842	0.8409	0.8499	0.8749	0.8623	6
11	0.7897	0.9306	0.9133	0.8388	0.8662	5
12	0.0000	0.9433	0.9406	0.8967	0.0000	46
13	1.0000	0.6756	0.6458	0.9104	0.7939	24
14	0.9219	0.7349	0.7147	0.8594	0.8031	20
15	0.9554	0.8034	0.8120	0.8211	0.8458	9
16	0.8633	0.9174	0.9133	0.6239	0.8196	18
17	0.8165	0.9554	0.9406	0.6943	0.8448	11
18	0.7598	0.9785	0.9657	0.8633	0.8873	2
19	1.0000	0.7349	0.7147	0.7598	0.7948	23
20	0.9858	0.7825	0.7909	0.7871	0.8325	13
21	0.8633	0.8409	0.8120	0.7922	0.8267	15
22*	0.9219	0.9554	0.9657	0.7419	0.8913	1
23	0.8842	0.9894	0.9889	0.0000	0.0000	46
24	0.5774	1.0000	1.0000	0.6943	0.7957	22
25	0.0913	0.9738	0.9713	0.9298	0.5323	35
26	0.0000	0.9684	0.9801	0.9329	0.0000	46
27	0.0000	0.9636	0.9832	0.9360	0.0000	46
28	0.0000	0.9612	0.9842	0.9391	0.0000	46
29	0.0000	0.9603	0.9845	0.9391	0.0000	46

30	0.0000	0.9601	0.9848	0.9391	0.0000	46
31	0.0000	0.9598	0.9848	0.9391	0.0000	46
32	0.0000	0.9598	0.9848	0.9391	0.0000	46
33	0.0000	0.9623	0.9762	0.9267	0.0000	46
34	0.0000	0.9646	0.9823	0.9329	0.0000	46
35	0.0000	0.9637	0.9837	0.9360	0.0000	46
36	0.0000	0.9625	0.9842	0.9360	0.0000	46
37	0.0000	0.9617	0.9844	0.9391	0.0000	46
38	0.0000	0.9611	0.9847	0.9391	0.0000	46
39	0.0000	0.9607	0.9847	0.9391	0.0000	46
40	0.0000	0.9603	0.9848	0.9391	0.0000	46
41	0.5374	0.9864	0.9834	0.9202	0.8322	14
42	0.3738	0.9842	0.9839	0.9329	0.7623	28
43	0.2475	0.9798	0.9821	0.9360	0.6871	32
44	0.1535	0.9757	0.9811	0.9360	0.6090	33
45	0.0913	0.9724	0.9812	0.9360	0.5344	34
46	0.0000	0.9698	0.9819	0.9360	0.0000	46
47	0.0000	0.9676	0.9828	0.9360	0.0000	46
48	0.0000	0.9657	0.9835	0.9360	0.0000	46
49	0.4894	0.9998	0.9996	0.8071	0.7926	25
50	0.5008	0.9997	0.9995	0.8554	0.8089	19
51	0.5297	0.9995	0.9991	0.8823	0.8266	16
52	0.5607	0.9989	0.9985	0.9002	0.8423	12
53	0.5758	0.9977	0.9971	0.9137	0.8506	8
54	0.5571	0.9956	0.9946	0.9235	0.8448	10
55	0.4941	0.9921	0.9911	0.9298	0.8198	17
56	0.3914	0.9876	0.9873	0.9329	0.7725	27

\*The double ring electrode-based argon cold plasma jet operating conditions corresponding to the highest composite desirability.

5. 3. Combinatorial Effects of Supply Voltage and **Supply Frequency on the Responses** To visually analyze the effects of SV and SF on the output parameters, Figure 7 presents the 3D surface plots of the experimental responses, PDC, JLwS, JLwoS and P with respect to variations in SV and SF. From Figure 7(a), it is observed that, PDC increases from 100 mA to 200 mA with increase in SV from 3.5 kV to 6 kV. However, the effect of SF appears to be more nonlinear with peaks observed near 15 kHz and 25 kHz. The effects on JLwS and JLwoS are more straightforward (Figure 7(b) and (c)). Both JLwS and JLwoS are found to increase with rise in SV and SF, both as individual and interaction effects, yielding a maximum of  $\geq 25$  mm at the highest values of SV and SF. Another observation is that, SV has a greater influence than SF on both JLwS and JLwoS. The power consumption (P) reaches a minimum of



Figure 6. (a) Main effect plot and (b) contour plot of composite desirability with respect to SV and SF

around 0.3 W at the minimum values of both SV and SF (Figure 7(d)). Comparing the effects of the two control parameters, it is found that, SF induces a greater change in P compared to SV.





**Figure 7.** 3D surface plots showing the contours of responses: (a) PDC, (b) JLwS, (c) JLwoS, (d) P, with respect to the variations in the control parameters: SV and SF

#### 6. CONCLUSIONS

This work presents a modeling and optimization methodology for the performance of the double ring electrode-based argon cold plasma jet using ANN and DFA techniques. The feedforward backpropagation ANN model with '2-8-20-4' topology using the Levenberg-Marquardt algorithm and tansig activation function accurately described the experimental responses of pulse discharge current, jet length with and without sleeve, and power consumption ( $R^2 > 0.96$ ) throughout the experimental range:  $3.5 \text{ kV} \le \text{SV} \le 6 \text{ kV}$  and 10 kHz $\leq$  SF  $\leq$  25 kHz. The optimization using DFA revealed that SV = 5 kV and SF = 25 kHz yielded the best multiresponse performance of PDC = 128 mA, JLwS = 25 mm, JLwoS = 22 mm and P = 0.97 W. The interaction effect analysis of composite desirability index showed that SV < 6 kV is advisable for a good performance (CDI > 0.6) for the entire range of 10 kHz  $\leq$  SF  $\leq$  25 kHz. The analysis of combinatorial effects of SV and SF showed that JLwS and JLwoS become maximum at SV = 6 kVand SF = 25 kHz. PDC becomes minimum near SV = 3.5kV and 15 kHz  $\leq$  SF  $\leq$  25 kHz, and P is minimized at SV = 3.5 kV and SF = 10 kHz. The findings of this study demonstrated that the proposed ANN model can be used to evaluate, obtain insights on, and predict the performance of the double ring electrode-based argon cold plasma jet. The results of this study would serve as

a benchmark for development of such fundamental predictive models for various types of cold plasma technologies and their optimization.

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## 8. APPENDIX

The results of various trails conducted to obtain the best accuracy ANN structure (shown in bold) are shown in Table 4. For additional quantitative comparison, the error metrics mean square error (MSE) and mean absolute percentange error (MAPE) have been included:

$$MSE = \frac{1}{n} \sum \left( y - \overline{y} \right)^2 \tag{8}$$

$$MAPE = \frac{100\%}{n} \sum \left| \frac{y - \overline{y}}{y} \right|$$
(9)

where, n is the number of data points, y and  $\overline{y}$  are the actual and predicted output value, respectively.

TABLE 4. Errors with different ANN structures

Neurons in Layer 1	Neurons in Layer 2	<b>R</b> <sup>2</sup>	MSE	MAPE (%)
20	3	0.62	37.119	25.52
18	6	0.76	30.234	19.35
16	8	0.77	27.292	19.01
14	12	0.82	25.632	15.67
12	14	0.91	20.246	9.13
10	16	0.90	20.842	10.02
8	20	0.97	16.062	3.62
6	20	0.89	21.423	10.34
3	20	0.71	31.357	21.35

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## Persian Abstract

#### چکیدہ

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پلاسمای فشار اتمسفر سرد (CAP) یک فناوری بسیار قوی و تاثیرگذار است که هم برای کاربردهای تکنولوژیکی و هم برای کاربردهای زیست پزشکی اجرا شده است. این مقاله بر اجرای شبکه عصبی مصنوعی (ANN) برای پلاسمای فشار اتمسفر سرد مبتنی بر الکترود دو حلقه جدید متمرکز است که برای کاربرد آن در زمینه زیست پزشکی فقط در منطقه تخلیه درخشش عمل میکند. ANN ذاتاً به تجسم پارامترهای خروجی مؤثر مانند جریان دبی اوج، توان مصرفی، طول جت (با آستین) و طول جت (بدون آستین) برای مجموعه پارامترهای ورودی ولتاژ و فرکانس منبع تغذیه با استفاده از مدل یادگیری ماشین کمک میکند. قابلیت مدل ANN با پیشبینی پارامترهای خروجی ACP فراتر از محدوده تجربی نشان داده میشود. در نهایت، تنظیمات بهینه ولتاژ تغذیه و فرکانس منبع تغذیه با استفاده از رویکرد تابع مطلوبیت ترکیبی تعیین میشود تا همزمان جریان تخلیه پیک، طول جت (با آستین) و طول جت (بدون آستین) را به حداکثر برساند و مصرف برق را به حداقل برساند.



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# Physical, Mechanical, and Thermal Properties of Polyvinyl Alcohol/Nanocrystalline Cellulose Bioplastic Film

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#### ABSTRACT

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Keywords: Bioplastic Film Nanocrystalline Cellulose Polyvinyl Alcohol The bioplastic film based on Polyvinyl Alcohol (PVA) for food packaging has been widely developed because of its biodegradable properties and safety. Nanocrystalline cellulose (NCC) is used as filler to improve mechanical strength. This study investigated how adding NCC into PVA films affects the physical, mechanical, and thermal properties. Combine acid hydrolysis 46 wt.% and ultrasonication process success to isolate commercial microcrystalline cellulose (MCC) became nanocrystalline cellulose (NCC). It has been characterized by x-ray diffraction (XRD), Fourier Transform Infrared (FTIR), Transmission Electron Microscope (TEM), Differential Scanning Calorimetry (DSC), and Thermal Gravimetric Analysis (TGA). NCC with needle shape form with an aspect ratio (L/D) of 12.4 has been high crystallinity index (76.4%). Addition of 6 wt.% NCC into PVA film improves the tensile strength and elongation by 35.30 MPa and 65.54%, respectively. The bioplastic film gives a barrier on the UV rays by 75% and still has good transparency. The thermal stability improves, indicated by the glass transition temperature (T<sub>g</sub>) increase from 109 to 114°C and maximum temperature (T<sub>max</sub>) from 275 to 300 °C.

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## **1. INTRODUCTION**

Chemical treatment is one of the methods to isolate the cellulose nanocrystal. The treatment was carried out using hydrolysis by adding a sulfuric acid solution (H<sub>2</sub>SO<sub>4</sub>). The purified fiber has been done to minimize the hemicellulose and lignin content before the acid hydrolysis process. The acid hydrolysis aims to fibrillate and open bundle micro cellulose to nanocellulose. Several previous research like Morais et al. (1) isolated cotton fibers by adding a sulfuric acid solution (60 wt.%) in a bath a stirred at 200 rpm at a temperature of  $45^{\circ}$ C for one hour. It is successfully producing the nanocrystalline

cellulose (NCC) with 12 nm of diameter and 177 nm of length. The aspect ratio (L/D) of NCC cotton is 19. Ghasemi et al. (2) have purified linter pulp followed by ultrafine grinder results the 30-70 nm of nanocellulose fiber's (NCF) diameter. The crystallinity index of nanocellulose is lower than purified fiber, it decreases from 79.5% to 65%. This phenomenon causes the decreased stability thermal of NCF from 280 to 240°C. Tonoli et al. (3) isolated the eucalyptus pulp sheets with the same concentration at 45°C for 30 minutes to produce nanocrystalline cellulose with diameters and lengths of 30 and 200 nm, respectively. Jiang and Hsieh (4), isolated rice straw by adding a sulfuric acid solution (64 wt.%) at

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preheat temperature 45°C for 45 minutes to produce NCC with 6.4  $\pm$  1.8 nm of diameter and 113  $\pm$  70 nm of diameter. Johar and Ahmad (5), isolated rice husks using a sulfuric acid of 10 mol/L at a preheat temperature of 50 °C for 40 minutes to produce NCC with 20 nm of diameter and 300 nm of length. It has an aspect ratio of 15. The aspect ratio depends on fiber resource, purified method, and fibrillated method. It is important to determine the NCC mechanical properties as filler in the polymer (6-9). Terzioglu and Parin (10) investigated the effect of adding lemon peel from 1 to 8 wt.% in the PVA (polyvinyl Alcohol)-starch biocomposite film. The mechanical strength increases by adding 1 wt.% lemon peel, showing good dispersion. The tensile strength increases from 24 to 25 MPa, whereas elongation rises from 260 to 275%. It is adding 2-8 wt. % causes aggregation in high concentration and starting to appear some voids in the matrix PVA-starch, it generates decreases in mechanical strength. Li et al. (11) developed bioplastic film combined the PVA 5 wt.%, it added by nanowhisker (CNWs) by 1 cellulose wt.%. concentration. The tensile strength and elongation PVA/CNWs bioplastic film are rises from 80 to 175 MPa and 170 to 330%, respectively. NCC's filler is known for high moisture absorption which leads to hydrophilic properties. To overcome this problem adding the biocompatible polymer is necessary to remove the reactivity of hydroxyl groups in the nanocellulose. The hydrophilic synthetics polymer, such as PVA, is easily dissolved in water, biodegradable, resistant to chemical conditions, and is an attractive material used for advanced applications. Furthermore, PVA is non-toxic to the human body, drug delivery systems, barrier materials, membranes, and yarn for surgery (12). Polymers can be degraded in two ways that are photodegradable or biodegradable. One definition of biodegradable polymer requires that the primary degradation mechanism is the result of the action and metabolism of microorganisms. Biodegradation can occur in either an aerobic or anaerobic environment. PVA is widely used as a sustainable plastic in the food industry because it is biodegradation; on the other hand, it has many advantages like high strength, good elasticity, lightweight, transparent, heat stable, and antimicrobial (13, 14).

This research aims to investigate the effect of adding NCC into PVA bioplastic film on mechanical and physical properties. There are several parameters and characteristics of NCC biocompatible with PVA bioplastic composites like aspect ratio (L/D), volume fraction ( $%V_f$ ), and homogenized suspension (15). This research investigates commercial microcrystalline cellulose (MCC) isolated by sulfuric acid hydrolysis. The physical tests were carried out in this study, including evaluation of TEM (transmission electron microscope), SEM (scanning electron microscope), XRD (x-ray

diffraction), FTIR (Fourier transform infrared), and Transmittance UV-Vis (Ultraviolet and Visible). The mechanical properties were tested through the tensile strength and then finally, the thermal stability was evaluated through TGA (thermal gravimetry analysis).

## 2. MATERIAL AND METHODS

**2. 1. Materials** Nanocrystalline cellulose was isolated from commercial microcrystalline cellulose (MCC) MERCK serial number 1.02330.0500, polyvinyl alcohol (PVA) fully hydrolyzed with 89-98 molecular weight from Sigma-Aldrich, sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) purity 96% from Sigma Aldrich, Sodium Hydroxide (NaOH) purity 98% and distilled water. The tools used are a burette tube, clamp burette, Bekker glass, magnetic stirrer, pH meter, centrifuge, and ultrasonic homogenizer 12 mm diameter and the power set is 240W.

**2. 2. Acid Hydrolysis** Acid hydrolysis of the commercial MCC is isolated by sulfuric acid 46 wt.%  $H_2SO_4$  with burrete tube into Erlenmeyer tube. The ratio of MCC powder and solution in the Erlenmeyer tube is 1:100. It was agitated at 350 rpm and preheated at 60°C for one hour by a magnetic stirrer. The acid hydrolysis process aims to break the cellulose chain into individual cellulose. The hydrolysis process starts by breaking the oxygen bonds in the  $\beta$ -1,4-Glycosidic chain, then the glycosidic ring bonds reacted with H<sub>2</sub>O molecules. Cellulose increased surface area and rise the hydroxyl group content. Figure 1 shows intramolecular reaction the decomposition of substances in chemical reactions caused by H<sub>2</sub>SO<sub>4</sub> and H<sub>2</sub>O molecules.

The acid suspension in the ice bath could stop the ionized process. Then it is gently dropped the sodium hydroxide NaOH with the same concentration by 46 wt.% into the acid suspension. Furthermore, centrifugation helps rinse the suspension for five cycles until neutral (pH=7). The NCC suspension was ultrasonicated for 15 minutes with a power of 240 watts and set the temperature at 60°C. It aims to get a homogenized suspension of NCC (16, 17).



Figure 1. Scheme of chemical reaction of acid hydrolysis and nanocellulose

**2. 3. Fabrication of PVA+NCC Bioplastic Film** The fabrication of bioplastic films with different weight of NCC. Firstly, prepare the PVA powder with a 3 wt.% (density is 1.19 g/cm<sup>3</sup>) and distilled water. It was mixed and heated constantly at 500 rpm at a temperature of 100°C for one hour.

The PVA suspension was put into the desiccator with silica gel for one night until the bubble was gone. Secondly, the NCC gel has weight by 0, 3, and 6 wt.%, and it was mixed into the PVA solution. The PVA suspension is mixed with NCC gel at a temperature of 50°C, stirred at 350 rpm for 30 minutes, followed by an ultrasonication of 240 watts for 15 seconds, 6 times. The last, it was poured into a hot Teflon plate at a temperature of 60°C for 4 hours to get a bioplastic composite film. The schematic process and production steps of the bioplastic composite are shown in Figure 2.

**2. 4. Morphology Analysis** The dimension of cellulose, nanocellulose, and surfaces of bioplastic composite have been identified by SEM (JSM-6510, LA-JEOL) and TEM (JEM-1400). The SEM photo can be detected surfaces solid material on the micro scale from 50 to 20,000 magnification. The voltage of SEM was set to 40 kV. The specimen has been coated with Au and used a sputtering method. The voltage of TEM is set at a range of 20 to 110 kV to get an excellent image contrast. NCC diameter (D) and length (L) were calculated by image-J software to results in the aspect ratio. The TEM photo can be detected nano scale material in the liquid suspension from 1000 to 300,000 magnification.

2. 5. XRD Analysis

The XRD diffraction patterns

for crystal structure are based on the scattering angle peaks and intensities of bioplastic composite. It was tested by using the Rigaku Miniflex-600 type which run at 40 kW, 15 mA, and CuK $\alpha$  radiation ( $\lambda$ =1.54060Å). The bioplastic film test sample was scanned in 2 $\theta$  range from 2° to 40° with a scan speed by 4° min<sup>-1</sup> and sampling pitch 0.02°. The solid structure of bioplastic film has a crystal and amorphous structure which is determined by crystallinity index according to Segal Equation 1.

$$CI = \frac{I_{110} - I_{am}}{I_{110}} \tag{1}$$

where  $I_{110}$  is a semi-crystalline structure plane at a scattering angle on the  $2\theta$ =19.8°, and  $I_{am}$  is an amorphous structure at a scattering angle on the  $2\theta$ =16°.

**2. 6. FTIR Analysis** FTIR is an analytical test method used to identify organic polymeric materials. The product composition analysis method with FTIR uses infrared light to scan the test sample and observe its chemical properties. It is used in the analysis to transmit infrared radiation from the sample test by absorbing and passing some of it through radiation. It measured wavenumber spectra from 4000-400 cm<sup>-1</sup> with a Shimadzu 8400S Spectrometer. Thin pellet samples were prepared with the help of potassium bromide (KBr).

**2. 7. UV-VIS Analysis** The transparency and ultraviolet barrier bioplastic composites were identified by spectrophotometer with Ocean optics USB-4000 of UV-Vis (ultraviolet-visible) obtained by continuously changing the wavelength of light. It is which separately passes through the test sample.



Figure 2. Scheme of fabrication of PVA+NCC bioplastic film



Figure 3. The photo of (a) MCC by SEM, (b) NCC by TEM



Figure 4. Surfaces morphology of bioplastic film: a) Neat PVA, b) PVA+NCC3%, and c) PVA+NCC6%

In an array spectrometer, light with a full wavelength that passes through the test sample is diffracted by a reflection and then received by the detector. As a result, it can provide a complete scan spectrum by 200–800 nm.

**2.8. Mechanical Analysis** The mechanical analysis used the tensile test of ASTM D-882 for thin plastic sheets, including film less than 1 mm. The paper test specimen is 100 mm in overall length; the specimen test is 25 mm gage length and 5 mm in width. The UTM (universal testing machine) by Pearson Panke Equipment Ltd has a maximum load of 400 N and a set cross-head speed of 2 mm/minute.

**2.9. TGA Analysis** The TGA (Thermogravimetric Analyzer) Mettler Toledo can run on a single temperature program (a constant heat rate at  $10 \circ C/min$  from 30 to  $600 \circ C$  with a nitrogen gas flow rate of 60 mL/minute). The bioplastic composite sample was tested in thin sheet film with a weight of 10 mg. Thermal degradation can be used to generate polymer degradation at different temperatures. Some examples of mass change processes are decompositions and oxidations. On the other hand, the TGA curve data are coupled with a derivative thermogram (DTG) curve to give the results better.

**2. 10. DSC Analysis** The Thermal degradability of bioplastic film can be calculated with DSC (Differential Scanning Calorimetry). DSC is one of the necessary tests to determine how much the energy a bioplastic film absorbs or release. This thermal analysis measures the heat energy absorbed and emitted by the test sample as a function of time and temperature. The glass temperature occurs when the material changes from the semi-liquid to the liquid phase  $(T_g)$ . The final melting temperature occurs when most of the liquid has been burned  $(T_m)$ . The gas used is nitrogen  $(N_2)$  with an average flow rate (flow rate) of 10 ml/minute at a temperature range of 30-300°C.

## **3. RESULT AND DISCUSSIONS**

**3.1. Morphology Analysis of NCC** Figure 3a shows the morphology of MCC was investigated by SEM (Scanning Electron Microscope), and it found that the diameter of MCC is  $\pm 20 \ \mu$ m. Figure 3b shows NCC by acid hydrolysis process combined with ultrasonication. The NCC has a diameter and length of around 25 nm and 310 nm with aspect ratio 12.4. Furthermore, other similar research by Krishnadev et al. (18) has been isolated Agave americana fiber by chemical extracted by 4 wt.% NaOH in hot water 80°C for two hours followed by bleaching treatment using 2 wt.% NaClO<sub>2</sub> in hot water 80°C for 4 hours and It's followed by acid hydrolysis with a nitric acid solution of 70% and acetic acid of 80% at a hot temperature 100°C for 30 minutes. Its morphology results in that the NCC has a diameter of  $18.2 \pm 10$  nm by TEM.

**3. 2. Morphology Analysis of Bioplastics Film** Figure 4a shows the morphology of PVA bioplastic composite products without addition of NCC. The surface morphology of bioplastic composites looks likes smooth and clear. Addition of NCC in the PVA bioplastic composite resulted in intermolecular cross-linked chemical bonds between NCC and PVA. It shows a little wrinkle spread on the surface structure (Figure 4b). Figure 4c shows big wrinkle spread well on the surfaces of the PVA matrix.

**3. 3. XRD Analysis of Bioplastic Film** Figure 5 shows the value of the crystallinity of bioplastic composites. The reference value in the crystallinity area with a value of  $2\theta$ =19.8° (plane 110) and the amorphous area at a value of  $2\theta$ =16°. Plane 110 of bioplastic film materials corresponding to d spacing 4.4801 Å, and it indicates the semi-crystalline typical structure (19, 20). The NCC's crystallinity by 76.4% higher than commercial MCC (Sigma Aldrich) by 74.8% (16). Adding NCC in the PVA impacted the bioplastic film crystallinity raises fraom 48.7% to 65.1%.

The crystallinity index of Neat PVA, PVA+NCC 3%, and PVA+NCC 6% there are 48.7%, 62.0%, and 65.1%, respectively. The crystallinity and amorphous intensity summarized in Table 1. Ilyas et al. (21) isolated the palm fiber by chemical purification followed by hydrolysis of 60 wt.% sulfuric acids, 45°C intermolecular for 45 minutes. The results of this treatment process increased the crystallinity index value from raw fiber to NCC from 55.8% to 85.9%.



Figure 5. XRD diffraction of bioplastic film

The selection of concentration, time, and temperature parameters for acid hydrolysis determine the aspect ratio of NCC. Aspect ratio (L/D) and crystallinity indexed are important parameters to determine mechanical properties.

**3. 4. FTIR Analysis** Figure 6 shows the bioplastic films' wavenumber spectra region in four main areas. The relative content of functional groups or groups of atoms in the material was estimated by intensity ratio of optical density (22). The first wavenumber is 3490 cm<sup>-1</sup>, it indicates O-H stretching (23). The NCC's hydroxyl make intermolecular cross-link bonded to PVA's hydroxyl (-OH) which is shown in Figure 7. It indicates by the peak

TABLE 1. Crystallinity index of bioplastic films

Samples	<b>I</b> <sub>110</sub> (2θ=19.8°)	$I_{\text{amorphous}}(2\theta=16^{\circ})$	<b>CI</b> (%)
Neat PVA	158	81	48.7
PVA+NCC 3%	308	117	62.0
PVA+NCC 6%	395	138	65.1



Figure 6. FTIR wavenumber spectra of bioplastic film



Figure 7. Schematic of intermolecular bond between PVA and NCC

of PVA+NCC sharper than neat PVA. The second area wavenumber region is 2931 cm<sup>-1</sup>, meaning that the C-H stretching vibration. The third region is 1627 cm<sup>-1</sup>, showing the O-H bending vibration means adsorbed of H<sub>2</sub>O (water vapor) content. It indicates that NCC material is suitable for combination with the same hydrophilic properties as PVA (24). The four region is 1190 cm<sup>-1</sup>, showing the asymmetric stretching vibration C-O-C indicates the glucose ring structure of cellulose (25).

Adding more NCC into PVA decreases the water vapor permeability of bioplastic film. Another study using hydrophilic polymers besides PVA like a Polylactic Acid (PLA) developed by Mirabolghasemi et al. (26). It was found that addition of NCC causes a decrease in the value of water vapor permeability (H<sub>2</sub>O) content. The nano-scale of NCC homogeneous structure increases the crystallinity of bioplastic film material which inhibit the water vapor.

3.5. The UV-Vis Absorbance Figure 8 shows that addition of NCC to the PVA matrix decreases the transparency of the bioplastic composite. Neat PVA has excellent transparency, which means the visible light transmission by 70% on the 650 nm wavelength. Adding NCC in PVA increases the absorbance of The UV rays at 300 nm wavelength. UV-A has a long wavelength of 400 nm, and UV-B has a short wavelength of 300 nm (27). Figure 9 shows that small transmittance on the wavelength range 300-400 nm, it indicates the material has good blocking of UV rays. Adding NCC 3 and 6 wt.% in the PVA could be reduced 70% and 75% of UV-A rays compared to without NCC. Therefore, the bioplastic composite could reduce UV rays to be applied as packaging. The average transmittance of visible light neat PVA is 70%. Addition of 3 and 6 wt.% CNF caused the decreases in the transmittance light to 45% and 37%, respectively.

**3. 6. Mechanical Analysis** 

Figure 10 shows the

tensile properties and elongation at break of bioplastic films. The thickness of bioplastic film is 25-30 µm. Adding NCC as filler into the PVA could improve the performance of the bioplastic composite with more strength and elasticity than neat PVA. The interaction between NCC and PVA by intermolecular bonding of the hydroxyl functional group can raise the toughness of bioplastic composite. The tensile strength and elongation at break of neat PVA by 26.61 MPa and 46.95 %, respectively. Addition of 3 wt.% NCC slightly increases the effect by 35.30 MPa of tensile strength and 65.54% of elongation at break. Whereas adding 6 wt.% of NCC gives an excellent improvement in the tensile strength and elongation properties increase by 38.67 MPa and 84.06%. This condition shows that NCC provides a good stress distribution in the PVA bioplastic composite matrix. The other research by Fortunati et al. (28) has isolated the MCC (Sigma Aldrich) by hydrolysis by sulfuric acid 64 wt.% at a temperature of 45°C for 30 minutes. It was produced at 10 nm in diameter and 200 nm in length. Adding NCC 5wt.% as filler in the PVA bio-nanocomposite film has increased tensile strength and elongation at the break by 44.3% and 300%, respectively. Previous research using PVA polymer as the matrix was conducted by Yudhanto et al. (29) extracted NCC from Agave cantala fiber with a combination process of sulfuric acid hydrolysis by 44 wt.% at temperature 60°C for one hour followed by ultrasonication (240Watt, diameter probe is 12 mm, 30 minutes times). It produced 45 nm of diameter and 1975 nm (aspect ratio is 43.8) NCC. Adding 8 wt.% in PVA/NCC film results in the highest tensile strength of 76.7% and elongation at the break of 112%. Addition of NCC 10 wt.% results in agglomeration NCC, and it causes stress concentration and affects low tensile properties. Frone et al. (30) isolated MCC with ultrasonication (20 kHz, 19 mm diameter probe, 200 Watts) for 20 minutes. It produces the NCC 70-150 nm in diameter. Adding the NCC filler 5 wt.% in the PVA matrix increases the tensile strength by 39%.

**3. 7. Thermal Degradability Analysis** Thermogravimetric analysis (TGA) and corresponding derivative thermogravimetry (DTG) curves of the NCC is shown in Figure 11. It shows that the thermal stability of NCC is high. The weight mass loss could be divided into three stages.

The first stage is the evaporation of adsorbed water in the NCC and bioplastic composite before a temperature 100°C. The second stage started at 230-300°C, the initial degradation temperature ( $T_{onset}$ ). It degrades an amorphous material such as hemicellulose and lignin. It is similar to conducted research by Babu et al. (31), that lignin of *Phaseolus vulgaris* fiber (PVFs) content degrades in the same temperature range. The third stage is a maximum temperature  $(T_{max})$  of NCC by 325°C, the cellulose degradation temperature range of 322-347°C. Figures 12 and 13 are shown the TGA and DTG curves of bioplastic film. Adding NCC into PVA causes the crystalline structure functional groups in the NCC to be able to inhibit heat flow. Furthermore, another research by Wang et al. (32), adding NCC into PVA and UPy (Ureido-Pyrimidinone) causes a rise the thermal stability. Table 2 shows an increase in thermal stability in each variation of bioplastic composites. The initial and maximum degradation of neat PVA is  $253^{\circ}$ C (T<sub>onset</sub>) and  $275^{\circ}$ C (T<sub>max</sub>) which are shown in Figures 12 and 13.



Figure 8. Transparency of bioplastic film (a) neat PVA, (b) PVA+NCC3%, (c) PVA+NCC6%



Figure 9. UV-Vis. transmittance spectra of bioplastic film



Figure 10. Tensile properties of bioplastic films



Figure 11. TGA/DTG curves of Nanocrystalline Cellulose (NCC)



Figure 12. TGA curves of bioplastic film



Figure 13. DTG curves of bioplastic film

According Gan et al. (33), addition of NCC into polymer as matrix give rise to intermolecular bonding between it, which rise the elongation at break and improvement the glass transition temperature ( $T_g$ ), and  $T_{max}$ . The excellent bonding between hydrogen the filler

	TA	BL	Ξ2.	Thermal	stability	of NCC of	on TGA	and DTG tes	st
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Samples	Tonset (°C)	$T_{max}$ (°C)
NCC	295	330
Neat PVA	253	275
PVA+NCC3%	270	290
PVA+NCC6%	280	300

(NCC) and the matrix can be improvement the stability thermal of bioplastic film.

The data obtained from the DSC (Differential Scanning Calorimetry) test include the glass transition temperature ( $T_g$ ) and melting temperature ( $T_m$ ). The glass transition is the initial transition temperature of the change in the material phase, which is rigid glass to rubbery (ductile stretching), meaning that the higher glass temperature shows the bioplastic film more rigid and elastic. In Figure 14 shows adding NCC into PVA film raises the glass temperature ( $T_g$ ) from 109 to 114°C



Figure 14. DSC curves of bioplastic film

and melting temperature ( $T_m$ ) from 195 to 233°C. The enthalpy (H) on meting point shows that the high absorbs energy need to degrades the PVA+NCC 6 wt.% by 158.1 J/g. The neat PVA only absorbs energy by 30.7 J/g, it was caused the neat PVA film degrades earlier at the glass temperature ( $T_g$ ).

#### 4. CONCLUSION

NCC has been isolated from MCC was successful in combining acid hydrolysis and ultrasonication. The resulting NCC measures 25 nm in diameter and 310 nm in length with an aspect ratio of 12.4. The addition of 6 wt.% NCC into PVA increased the tensile strength and elongation at the break by 45.3% and 79.0%, respectively. The good mechanical strength correlated with the high crystallinity index by 65.1%. In addition, the TGA/DTG for maximum temperature (T<sub>max</sub>) increases from 275 to 300°C. The DSC test shows rising the heat enthalpy and transition glass temperature  $(T_g)$ , from 134.4 J/g (109 °C) to 154.8 J/g (114°C). It indicates adding NCC improving the thermal stability. The transparency properties are still good, and it was excellent barrier of UV rays by 75%. It's suitable to be applied to plastic packaging.

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#### Persian Abstract

چکیدہ

فیلم بیوپلاستیک مبتنی بر پلی وینیل الکل (PVA) برای بسته بندی مواد غذایی به دلیل خواص زیست تخریب پذیر و ایمنی آن به طور گسترده توسعه یافته است. سلولز نانو کریستالی (NCC) به عنوان پرکننده برای بهبود استحکام مکانیکی استفاده می شود. این مطالعه بررسی کرد که چگونه افزودن NCC به فیلمهای PVA بر خواص فیزیکی، مکانیکی و حرارتی تأثیر میگذارد. ترکیب هیدرولیز اسید ٤٦ درصد وزنی و موفقیت فرآیند فراصوت برای جداسازی سلولز میکروکریستالی تجاری (MCC) به نیلم این به طور گسترده برای می و حرارتی تأثیر میگذارد. ترکیب هیدرولیز اسید ٤٦ درصد وزنی و موفقیت فرآیند فراصوت برای جداسازی سلولز میکروکریستالی تجاری (MCC) به سلولز نانوبلور (NCC) شد. با پراش اشعه ایکس (XRD)، تبدیل فوریه فروسرخ (FTIR)، میکروسکوپ الکترونی عبوری (TEM)، کالریمتری اسکن تفاضلی (OSC)، و آنالیز وزنی حرارتی (TGA) مشخص شده است. NCC با فرم سوزنی شکل با نسبت ابعاد 21/4 (L/D) دارای شاخص کریستالینیتی بالا (۲۷۶ درصد) بوده است. افزودن ٦ درصد وزنی حرارتی (TGA) مشخص شده است. NCC با فرم سوزنی شکل با نسبت ابعاد 21/4 (L/D) دارای شاخص کریستالینیتی بالا (۲۷۵ درصد) بوده است. افزودن ٦ درصد وزنی حرارتی (TGA) مشخص شده است. NCC به فرو را به ترتیب ۳۵.۳۰ می ایکترونی عبوری (نام هیلم ۱۹۷۹) می درصد) بوده است. افزودن ٦ درصد وزنی حرارتی (TGA) مشخص شده است. NCC به فرو را به ترتیب ۳۵.۳۰ می می دوسکوپ الکترونی می در می تلینیتی بالا (۲۰۷ درصد) بوده است. افزو دن ٦ درصد وزنی حرارتی (TGA) می PVA استحکام کششی و ازدیاد طول را به ترتیب ۳۵.۳۰ می ایند که با افزایش دمای انتقال شیشه ای (Tg) از ۲۰۹ به ۱۹۶ درجه سانتی گراد و دراکش ماوراء بنفش ایجاد می کند و همچنان شفافیت خوبی دارد. پایداری حرارتی بهبود می یابد که با افزایش دمای انتقال شیشه ای (Tg) از ۲۰۰ به ۱۹۰ به ۱۹ درجه سانتی گراد و داند.


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# Seismic Vulnerability of Irregular Reinforced Concrete Buildings Considering the Soil-structure Interaction

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ABSTRACT

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Keywords: Plastic Hinges Seismic Response Fragility Curves In this study, we present an investigation into the seismic vulnerability assessment of medium-rise reinforced concrete structures featuring vertical geometric irregularity (setback). We considered the effects of the percentage and location of the setback along the height of the building, as well as the impact of changing site classes. Additionally, we incorporated the effects of soil-structure interaction into the nonlinear response of the building. In the first part, we investigated the influence of the aforementioned parameters on the seismic response of a structure through nonlinear static analyses. We analyzed the capacity curves and the development of plastic hinges in the structural elements. In the second part, we analyzed the seismic fragility of building frames using a probabilistic study approach. We developed fragility curves to assess the vulnerability of the structures. In conclusion, the obtained results highlight the fundamental importance of considering structural irregularities as well as the impact of different site classes on the seismic vulnerability of buildings.

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NOMENC	NOMENCLATURE				
μ	The ultimate ductility	T	Period of the flexible-base structure		
G	Shear modulus of the soil	ρ	Density		
$G_0$	Initial shear modulus	$D_y$	Elastic displacement		
L	Length of the foundation	$V_y$	Elastic shear velocity		
В	Width of the foundation	If	Moment of inertial		
υ	Poisson's ration	A <sub>f</sub>	The area of foundation		
ĩ	Total system damping	$r_u = \sqrt{\frac{A_f}{\pi}}$	The foundation radii of translation		
ε <sub>f</sub>	Damping of the foundation	$r_{\theta} = \sqrt[4]{4 \times I_{\rm F}/\pi}$	The foundation radii of rotation		
ε	Damping of the structure	$K_{u} = \frac{8}{2-\nu} \times G \times r_{u}$	The static stiffness of a disk on a half- space for translational deformation modes		
Т	Period of the fixed-base structure	$K_{\theta} = \frac{8}{3(1-\nu)} \times G \times r_{\theta}$	The static stiffness of a disk in a half- space for rotational deformation modes		
Du	The ultimate displacement				

#### **1. INTRODUCTION**

Research into vertical irregularities in buildings has been an active field of study since the 1970s. Several researchers have played a pioneering role in this field. Chopra and Kan (1) focused their study on the seismic response of eight-storey buildings, subjecting them to seismic ground motion data.

Similarly, Ruiz and Diederich (2) carried out analytical studies on models of five- and twelve-storey buildings with irregularities in resistance. The impact of building setback on the seismic response of multi-storey structures was assessed by Shahrooz and Moehle (3).

Valmundsson and Nau (4) undertook a parametric

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study of two-dimensional building structures with irregularities in mass, stiffness and strength. Their results indicate that strength irregularities have the most significant influence on response compared to mass and stiffness irregularities.

In another relevant study, Michalis et al. (5) examined the effect of vertical irregularities on the capacity of a 9storey building using incremental dynamic analysis (IDA). They concluded that irregularities have a substantial impact on boundary states and depend on earthquake intensity.

As for Shaikh and Shinde (6), their interest focused on the seismic response of a reinforced concrete frame presenting a vertical irregularity associated with a mass irregularity.

Furthermore, Shah et al. (7) carried out a study on the seismic risk assessment of mid-rise steel buildings, highlighting different types of vertical irregularities, such as mass, stiffness and/or resistance irregularities.

In a recent study, Kyoung et al. (8) proposed a simplified modeling method to examine the behavior of buildings with irregularities. Their approach consists of transforming vertically irregular structures into geometrically regular ones using a floor stiffness equation.

Also Hait et al. (9) confirmed that the buildings with irregular configurations suffer greater damage than those with regular contours, mainly due to the increased influence of torsional effects.

On the other hand, Mouhine and Hilali (10) assessed the seismic vulnerability of twenty building structures with vertical geometric irregularities at different positions. They adopted a probabilistic approach based on non-linear static analysis to calculate damage probabilities. The results revealed that the percentage of shrinkage has a significant impact on the dynamic response of irregular structures and modifies building performance.

As part of our research, we focused on studying the seismic behavior of reinforced concrete buildings with vertical geometric irregularities, taking into account soil-structure interaction. We carried out three-dimensional simulations of medium-sized building structures, including shrinkage, using SAP 2000 finite element analysis software.

#### 2. SOIL-STRUCTURE INTERACTION

**2. 1. Non-linear Approach for Assessing the Seismic Performance of Strutures** We introduce a simplified model tailored to address the intricate challenges posed by nonlinear soil-structure interaction (SSI). The N2 method, originally formulated by Fajfar (11), is employed to assess the nonlinear behavior of the structure. In its initial version, this method assumes a fixed structure base, thereby excluding the influence of soil-structure interaction (SSI). Our proposed approach, named the N2-SSI method, extends the N2 method to incorporate soil effects into the nonlinear response (12).

**2.2. Foundation Impedances** The deformations of the structure during seismic shaking are affected by the interactions among the three interconnected systems: the structure, the foundation, and the geological media underlying and surrounding the foundations.

When a structure is built on soft soil, it is generally more susceptible to significant deformations compared to if it were erected on rock soil. As a result, various issues can arise, such as cracking due to differential settlements (13, 14).

The consideration of soil-structure interaction is accomplished by integrating a system of springs and dampers. The foundation and its interaction with the soil (spring-dampers) are modeled using impedance functions. The expression for these foundation impedances is cited in Table 1 according to the FEMA 356 (15) standard.

**2. 3. Damping and the Effective Period of the Soilstructure System** Typically, a damping coefficient of 5% is employed in dynamic analyses for ordinary structures experiencing seismic forces. Nevertheless, this value holds limited significance for reinforced concrete buildings when considering Soil-Structure Interaction (SSI). Soil exhibits two forms of damping: internal damping caused by the soil's hysteresis (hysteretic damping), and damping resulting from the dispersion of seismic waves (radial damping).

To account for the increase in damping, Veletsos and Nair (16) propose the following similar Equation 1:

$$\tilde{\varepsilon} = \varepsilon_{\rm f} + \frac{\varepsilon_{\rm i}}{\binom{T^3}{(T^3)}} \tag{1}$$

In the given equation, the total system damping is calculated by adding the damping of the foundation to a

**TABLE 1.** Foundation impedances and total damping for the cases studied

Degrees of Freedom	Foundation impedances	
Translation along the x-axis	$K_{x} = \frac{GB}{2-\nu} \left[ 3.4 \left( \frac{L}{B} \right)^{0.65} + 1.2 \right]$	
Translation along the y-axis	$K_y = \frac{{}_{GB}}{2-v} \left[ 3.4 \left(\frac{L}{B}\right)^{0.65} + 0.4 \frac{L}{B} + 0.8 \right]$	
Translation along the z-axis	$K_z = \frac{GB}{1-v} \left[ 1.55 \left( \frac{L}{B} \right)^{0.75} + 0.8 \right]$	
Rotation about the x-axis	$K_{xx} = \frac{GB^3}{1-\nu} [0.4 \frac{L}{B} + 0.1]$	
Rotation about the y-axis	$K_{yy} = \frac{GB^3}{1-v} \left[ 0.47 \left( \frac{L}{B} \right)^{2.4} + 0.034 \right]$	
Rotation about the z-axis	$K_{zz} = GB^3 [0.53 \left(\frac{L}{B}\right)^{2.45} + 0.51]$	

portion of the structure's damping, which is typically assumed to be 5% for conventional structures.

When determining the effective period, we can combine the two expressions for the period, using both the fixed T (rigid foundation) and  $\overline{T}$  (flexible foundation) as bases (17), and it is easy to arrive at Equation 2:

$$\frac{\overline{T}}{T} = \sqrt{1 + \frac{K}{K_u} + \frac{K h_{eff}^2}{K_{\theta}}^2}$$
(2)

**2. 4. The Results of Foundation Impedances and Total Damping for the Soil-structure System Used** Table 2 displays the values of spring stiffness corresponding to different directions, based on the shear wave velocity of the soil for each given site category. These values are specific to a foundation with a section of 18.47x3 m<sup>2</sup>.

#### **3. DEVELOPMENT OF FRAGILITY CURVES**

Conducting a quantitative assessment of the likelihood of seismic damage under various seismic loads is crucial. In this context, seismic fragility analysis serves as a significant approach for evaluating the chances of structures or components surpassing a predefined damage threshold when exposed to progressively stronger seismic ground motions (18-22).

This method has been utilized to evaluate the susceptibility of diverse structures to seismic events.

Fragility curves represent the relationship between a specific seismic intensity parameter, such as peak acceleration, spectral intensity, or macroseismic intensity, and the estimated average damage value of a structure. These curves are utilized to evaluate the vulnerability of a particular building and estimate the potential damage it may experience in the event of an earthquake.

The fragility curve follows a logarithmic function in a normal distribution and can be described by the following Equation 4:

$$P(dsi/S_d) = \phi(\frac{1}{\beta_{dsi}} \times \ln\left(\frac{S_d}{S_{d,dsi}}\right))$$
(4)

where,  $\beta_{dsi}$  is the standard deviation of the logarithm of the spectral displacement of the damage state dsiand  $\phi$  is the normal distribution function.

Threshold values  $\overline{S_{d,ds_1}}$  are given as a function of Dy and the ultimate displacement Du of the structure. For  $\beta_{dsi}$  is calculated directly as a function of  $\mu_u$  (see Table 3):

# 4. THE GEOMETRIC CHARACTERISTICS OF THE STRUCTURES STUDIED

The following section focuses on quantifying the vulnerability of six reinforced concrete irregular

TABLE 2.	The foundation	tion imped	ances and	total	damping	for
the studied	cases.					

Total damping		Degrees of freedom	Foundation impedances (* 10 <sup>9</sup> N/m)
		translation along the x-axis 10 <sup>9</sup> N/m	18445.92927
		translation along the y-axis $10^9 \text{ N/m}$	26978.8793
		translation along the z-axis 10 <sup>9</sup> N/m	21565.30743
Soil A	5%	rotation about the x-axis 10 <sup>9</sup> N.m/rd	76129.92582
		rotation about the y-axis $10^9$ N.m/rd	980618.9313
		rotation about the z-axis 10 <sup>9</sup> N.m/rd	852367.2701
Soil B	5%	translation along the x-axis $10^9{ m N/m}$	88,86664316
		translation along the y-axis $10^9 \text{ N/m}$	129,975693
		translation along the z-axis $10^9 \text{ N/m}$	103,8948189
Soil B	5%	rotation about the x-axis 109 N.m/rd	366,769863
		rotation about the y-axis 109 N.m/rd	4724,31133
		rotation about the z-axis 109 N.m/rd	4106,435459
		translation along the x-axis 10 <sup>9</sup> N/m	12,9697263
		translation along the y-axis $10^9{ m N/m}$	18,96942546
Seil C	60/	translation along the z-axis $10^9 \text{N/m}$	15,16302762
5011 C	0%	rotation about the x-axis 10 <sup>9</sup> N.m/rd	53,5285746
		rotation about the y-axis 10 <sup>9</sup> N.m/rd	689,4940859
		rotation about the z-axis 10 <sup>9</sup> N.m/rd	599,3176075
		translation along the x-axis $10^9{ m N/m}$	1,045263868
		translation along the y-axis $10^9 \text{ N/m}$	1,528795178
Seil D	120/	translation along the z-axis $10^9 \text{ N/m}$	1,222027707
3011 D	13%	rotation about the x-axis 10 <sup>9</sup> N.m/rd	4,314006605
		rotation about the y-axis 109 N.m/rd	55,56811596
		rotation about the z-axis 109 N.m/rd	48,30055978

Damage status thresholdsDefinition $\beta_{dsi}$ The state of damage				
$\overline{Sd}_{ds1}$	0.7 D <sub>y</sub>	$\beta_{ds1} = 0.25 + 0.07 \ln{(\mu_u)}$	Light	
$\overline{Sd}_{ds2}$	Dy	$\beta_{ds2} = 0.2 + 0.18 \ln{(\mu_u)}$	Moderate	
$\overline{Sd}_{ds3}$	$D_y + 0.25 (D_u - D_y)$	$\beta_{ds3} = 0.1 + 0.4 \ln{(\mu_u)}$	Severe	
$\overline{Sd}_{ds4}$	D <sub>u</sub>	$\beta_{ds4} = 0.15 + 0.5 \ln{(\mu_u)}$	Complete	

buildings, in accordance with FEMA 440 (23) standards. The column dimensions are 30x30 cm<sup>2</sup>, and the beam dimensions are 25x30 cm<sup>2</sup>, with a floor height of 3 meters, as shown in Table 4. The buildings are also depicted in Figure 1.

The structure is subjected to a live load of 2  $kN/m^2$  and a dead load of 7  $kN/m^2.$ 

Table 5 presents the properties of four different types of soil on which the studied structures are founded. The SAP2000 software was used to conduct numerical studies.

#### **5. RESULTS AND DISCUSSION**

**5. 1. Capacity Curves and Plastic Hinge Development** Using nonlinear static analyses (24, 25), capacity curves have been constructed for structures

**TABLE 4.** Details of the structural elements

Type of structure	Type of section	Reinforcement	
Column	(30x30) cm <sup>2</sup>	127	12
Beam	$(25x^{2}0)$ cm <sup>2</sup>	Тор	Upper
Dealin	(25x50) thi	3T10	6T10



**Figure 1.** X-Z plan view of the studied construction models with vertical geometric irregularity

TABLE 5	. The	characteristics	of	the soil	s

Soil type	Description	G <sub>0</sub> (N/m) *10 <sup>6</sup>
Soil A	Rock soil	689475,6
Soil B	Hard soil	3321,675
Soil C	Soft soil	484,785
Soil D	Very soft soil	39,07008

S1-1, S1-2, and S1-3, as well as S2-1, S2-2, and S2-3, for each soil type, as illustrated in Figures 2-9. Subsequently, the development of plastic hinges in the structural elements of the six reinforced concrete buildings with irregularities has been examined.



**Figure 2.**The capacity curves for the studied building models for soil type A (S1-1;S1-2;S1-3)



**Figure 3.** The capacity curves for the studied building models for soil type A (S2-1;S2-2;S2-3)



**Figure 4.** The capacity curves for the studied building models for soil type B (S1-1;S1-2;S1-3)



**Figure 5.** The capacity curves for the studied building models for soil type B (S2-1;S2-2;S2-3)



**Figure 6.** The capacity curves for the studied building models for soil type C (S1-1;S1-2;S1-3)



**Figure 7.** The capacity curves for the studied building models for soil type C (S2-1;S2-2;S2-3)



**Figure 8.**The capacity curves for the studied building models for soil type D (S1-1;S1-2;S1-3)



**Figure 9.**The capacity curves for the studied building models for soil type D (S2-1;S2-2;S2-3)

**5.1.1. The Capacity Curves** Based on the nonlinear static analysis PUSHOVER, capacity curves were established for each building and each soil type, as shown in Figures 2-9. Using these curves, capacity spectra were defined, and elastic capacity points for the modeled reinforced concrete buildings were identified, as indicated in Table 6. The results presented in Table 7 reveal that the setback value and soil type have an influence on the elastic capacity of the building. A significant reduction of 16% is observed for the S1 model with soil types A and B, and a reduction of approximately 11% for the S2 model.

For soil type C, a significant reduction of 16.41% is observed for the S1 model, and a reduction of approximately 11% is observed for the S2 model.

For soil type D, a notable reduction of 14% is observed for the S1 model, and a reduction of approximately 13.5% is observed for the S2 model.

Table 6 reveals that the displacement corresponding to the performance point decreases with an increase in the setback value, particularly for soil types C and D. This indicates that the setback has an influence on the inelastic deformation capacity of the structure during an earthquake, which explains the observed reduction in seismic performance. Consequently, the ductility of the structure will be diminished, potentially leading to significant energy release and damage to the structural elements of the buildings.

0.14	Type of	Performance point		
Soil type	structure	V (kN)	D (mm)	
	S1-1	17.143	1.95	
	S1-2	16.486	1.93	
C - 11 A	S1-3	15.859	1.696	
5011 A	S2-1	18.804	1.825	
	S2-2	18.512	1.936	
	S2-3	18.274	1.676	
	S1-1	21.429	2.397	
	S1-2	20.607	2.345	
C-11 D	S1-3	19.823	2.072	
S011 B	S2-1	23.51	2.249	
	S2-2	23.129	2.355	
	S2-3	22.828	2.079	
	S1-1	20.293	2.273	
	S1-2	19.514	2.236	
6-1 C	S1-3	18.771	1.976	
5011 C	S2-1	22.262	2.124	
	S2-2	21.902	2.243	
	S2-3	21.616	1.978	
	S1-1	14.773	1.626	
	S1-2	14.201	1.7	
Soil D	S1-3	13.66	1.527	
2011 D	S2-1	16.19	1.43	
	S2-2	15.936	1.685	
	S2-3	15.727	1.512	

**TABLE 6.** Performance points for the studied buildings

**TABLE 7.** Elastic capacity of the studied buildings

Coll trung	Type of	Elastic capacity	
Son type	structure	Vy (kN)	Dy (mm)
	S1-1	181.51	19.12
	S1-2	178.76	18.28
Soil A	S1-3	166.43	15.97
5011 A	S2-1	185.75	16.92
	S2-2	228.89	20.82
	S2-3	173.11	15.11
	S1-1	181.51	19.1
	S1-2	178.76	18.28
Coil D	S1-3	166.43	16
2011 D	S2-1	185.77	16.91
	S2-2	228.85	20.86
	S2-3	172.20	15.09

S = 11 4	Type of	Elastic capacity		
Son type	structure	Vy (kN)	Dy (mm)	
	S1-1	181.16	19.13	
	S1-2	178.80	18.30	
Seil C	S1-3	166.51	15.99	
5011 C	S2-1	185.92	16.93	
	S2-2	228.91	20.88	
	S2-3	171.86	15.08	
	S1-1	178.56	18.89	
	S1-2	179.31	18.48	
Soil D	S1-3	167.37	16.24	
5011 D	S2-1	187.58	17.25	
	S2-2	229.54	21.08	
	S2-3	168.07	14.92	

5. 1. 2. Distribution of Plastic Hinges The finite element software SAP2000 offers the capability to visualize the development of plastic hinges in structural elements. This allows for tracking and analyzing the behavior of the structure when subjected to loads, particularly in identifying areas where plastic deformations occur and plastic hinges form. This functionality is crucial for evaluating the ductility of the structure and understanding its response to extreme loads, such as those generated by an earthquake. Figures 10-15 provide an illustration of the distribution of plastic hinges for each building on each soil type. They highlight the presence of plastic hinges in most of the columns on the first and second floors, as well as in some columns on the third floor. These images allow for visualizing the areas of plastic deformation and identifying the structural elements that experience the most significant deformations during an earthquake.



Figure 10. The development of plastic hinges in structural elements for the model S1-1



**Figure 11.** The development of plastic hinges in structural elements for the model S1-2



**Figure 12.** The development of plastic hinges in structural elements for the model S1-3



**Figure 13.** The development of plastic hinges in structural elements for the model S2-1

As the applied force and rotation of the plastic hinges increase, different types of hinges can be observed. For cases S1-1, S1-2, and S1-3 on soil types A and B, Type B, Type Intermediate Opening (IO), and Type C hinges are observed. This suggests the presence of damage in the



Figure 14. The development of plastic hinges in structural elements for the model S2-1



**Figure 15.** The development of plastic hinges in structural elements for the model S2-3

structure, but it is not yet considered to be very significant.

However, for soil types C and D, the appearance of Type D hinges is observed in addition to the other types mentioned earlier. This observation indicates the presence of more significant damage in the structure, requiring special attention.

These observations help in understanding the evolution of structural behavior and identifying the most vulnerable areas to damage during an earthquake.

By examining cases S2-1, S2-2, and S2-3, it is observed that for soil types A and B, Type B, Type IO, Type C, and Type D, hinges are formed. However, for soil types C and D, the appearance of Type E hinges is also observed, indicating a higher level of damage that could lead to structural failure.

These observations lead us to conclude that vertical geometric irregularities at different levels, as well as the soil type, have a negative influence on the behavior of the structure during an earthquake. Vertical geometric irregularities can result in stress concentration and an uneven redistribution of seismic forces, leading to zones that are more vulnerable to damage. Additionally, soil characteristics such as stiffness and the ability to dissipate seismic energy can also play a significant role in the overall behavior of the structure.

**5. 2.Curves of Fragility** The fragility curves are created through the compilation of seismic intensity values associated with a particular soil type until they align with a pre-established damage intensity threshold. These curves adeptly illustrate the propagation of seismic intensity influenced by variations in soil characteristics, highlighting a substantial likelihood of reaching or surpassing a notable level of seismic damage (26-28).

The vulnerability of a typical reinforced concrete structure will be analyzed using a seismic performance approach that integrates the effects of Soil-Structure Interaction (SSI) into the nonlinear response.

Fragility curves are constructed to assess the probability of exceeding different seismic intensities, as illustrated in Figures 16-19. The probability of exceeding is determined using Equation 4. The damages probabilities are shown in Figure 20; these are computed taking into account the performance points of each structure.

This approach allows for estimating the probability of experiencing different levels of damage based on the seismic intensity. It provides valuable insights to assess the vulnerability of the structure and make informed decisions regarding design and seismic strengthening.

Figure 20 displays the calculated damage probabilities for various construction models based on different site classes. The results emphasize the critical



Figure 16. Fragility curves for Soil A



Figure 17. Fragility curves for Soil B



Figure 18. Fragility curves for Soil C

significance of site selection in seismic vulnerability analysis.

Structures constructed on soil types A and B exhibit low damage probabilities, regardless of the damage state under consideration. Conversely, structures built on soil types C and D demonstrate higher damage probabilities. This trend remains consistent regardless of the setback position along the building height.



Figure 19. Fragility curves for Soil D



Figure 20. The effect of soil type on the seismic vulnerability of the studied models

It has been confirmed that the behavior of a structure is influenced not just by its motion characteristics and the specifics of the seismic forces it experiences, but also by the surrounding external conditions at its foundation. This encompasses the interplay between the structure, its base, and the underlying soil (29-31).

Furthermore, Figure 20 illustrates the considerable influence of shrinkage position on the probability of damage. As the building height increases, so does the likelihood of damage. In other words, the probability of damage rises as the shrinkage exceeds one storey.

These observations underscore the importance of considering both site selection and setback position when analyzing the seismic vulnerability of building structures (32). This comprehensive analysis provides a better understanding of the risks associated with different seismic scenarios and guides decisions on seismic design and strengthening. Incorporating these considerations is essential for enhancing the resilience of buildings against potential earthquakes.

#### **6. CONCLUSIONS**

The objective of this research was to investigate the impact of changing site class and incorporating Soil-Structure Interaction (SSI) effects on the structural vulnerability of irregular reinforced concrete buildings during earthquakes.

The main conclusions drawn from this study are as follows:

• Ultimate Capacity and Plastic Hinge Development:

The results of the study highlighted the influence of vertical geometric irregularity and changing soil class on the behavior of the structure. In the case of soft soil conditions, a significant decrease in the building's elastic capacity is evident. The S1 model displays a reduction of about 14%, while the S2 model shows an approximate reduction of 13.50%.

The development of plastic hinges in structural elements and the ultimate capacity of the building were notably affected. As the setback margin value increased, the structural fragility of reinforced concrete buildings also increased. Therefore, it can be concluded that the degree of vertical geometric irregularity has a significant impact on the performance of building structures. Higher irregularity values lead to a more pronounced reduction in inelastic deformation capacity.

• Damage Probabilities and Site Selection:

The calculated damage probabilities for different building models underscore the importance of site selection in seismic vulnerability analysis. Structures constructed on rocky soil exhibit low probabilities of damage, regardless of the considered damage state. In contrast, buildings erected on loose soil show higher probabilities of damage. • Significance of Site Class and Geometric Irregularity:

The research highlights that both site class and geometric irregularity are crucial factors influencing the seismic vulnerability of these structures. During the structural analysis phase, it is vital to take these aspects into account to better understand the associated risks and implement appropriate design and reinforcement measures.

Considering these findings, it becomes evident that a comprehensive seismic risk assessment should consider both site selection and geometric irregularity to ensure the safety and resilience of irregular reinforced concrete buildings during earthquakes. Properly accounting for these factors in the design and strengthening processes will lead to more effective mitigation strategies and safer structures.

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#### Persian Abstract

#### چکیدہ

در این مطالعه، ما تحقیقی در مورد ارزیابی آسیبپذیری لرزهای سازه های بتن مسلح با ارتفاع متوسط با بینظمی هندسی عمودی (پسرفت) ارائه میکنیم. ما تأثیرات درصد و مکان عقبنشینی در طول ارتفاع ساختمان و همچنین تأثیر تغییر کلاس های سایت را در نظر گرفتیم. علاوه بر این، ما اثرات برهمکنش خاک-ساختار را در پاسخ غیرخطی ساختمان گنجانده ایم. در بخش اول، تأثیر پارامترهای فوق بر پاسخ لرزهای یک سازه را از طریق تحلیل های استاتیکی غیرخطی بررسی کردیم. ما منحنی های ظرفیت و توسعه لولاهای پلاستیکی را در عناصر ساختاری تجزیه و تحلیل کردیم. در بخش دوم، شکنندگی لرزهای قابهای ساختمان را با استفاده از رویکرد مطالعه احتمالی تحلیل کردیم. ما منحنی های شکنندگی را برای ارزیابی آسیبپذیری سازهها ایجاد کردیم. در نتیجه، نتایج به دست آمده اهمیت اساسی در نظر گرفتن بی نظمی های سازهای و همچنین تأثیر طبقات مختلف سایت بر آسیبپذیری لرزهای ساختمان ما را برجسته میکند.

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## Formation Control and Obstacle Avoidance of a Multi-Quadrotor System Based on Model Predictive Control and Improved Artificial Potential Field

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#### PAPER INFO

#### ABSTRACT

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Keywords: Quadrotor Formation Control Model Predictive Control Obstacle Avoidance Improved Artificial Potential Field The purpose of this article is to control the formation and pass static and dynamic obstacles for the quadrotor group, maintain the continuity and flight formation after crossing the obstacles, and track the moving target. Model Predictive Control (MPC) method has been used to control the status and position of quadrotors and formation control. Flight formation is based on the leader-follower method, in which the followers maintain a certain angle and distance from the leader using the formation controller. The improved Artificial Potential Field (APF) method has been used to pass obstacles, the main advantage of which compared to the traditional APF is to increase the range of the repulsive force of the obstacles, which solves the problem of getting stuck in the local minimum and not passing through the environments full of obstacles. The results of the design of the attitude and position controller showed that the quadrotors were stabilized and converged in less than 3 seconds. Formation control simulations in the spiral path showed that the followers, follow the leader. The results of the quadrotors passing through the obstacles were presented in four missions. In the first mission, 4 quadrotors crossed static obstacles. In the second mission, 4 quadrotors crossed dynamic obstacles. In these two missions, the quadrotors maintained a square flight formation after crossing the obstacles. In the third mission, the number of quadrotors increased to 6. The leader tracked the moving target and the quadrotors crossing the static obstacles. In the last mission, the quadrotors passed through the dynamic obstacles and the leader tracked the static target. In these missions, the quadrotors maintain the hexagonal formation after crossing the obstacles. The results simulations showed that the quadrotors crossed the fixed and moving obstacles and after crossing, they preserved the flight formation.

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#### **1. INTRODUCTION**

Robots have been widely used in military and civilian fields such as anti-terrorism operations, identification, agriculture, etc. (1, 2). In addition, instead of using a single robot, multiple robots in a group formation can complete some complex missions without incurring high costs (3, 4). Among the controllers used to control the formation is model predictive control (MPC). MPC is a controller where optimization is solved online. The vital advantage of this method is considering a performance criterion and constraints. For multi-agent systems, the time of optimization calculations increases with the number of agents. To solve this problem, decentralized MPC (5, 6) or distributed MPC (7) have been proposed. The formation control of multiple robots is generally classified into leaderless and leader-follower (8). In the leaderless formation control problem, the robots are driven to a prescribed pattern at a certain speed. In contrast in the leader-follower control problem, the follower robots agree on the reference information of a leader while maintaining the defined pattern. In the control of leader-follower formation, the problem of the availability of information about the leader can be solved by distributed technique. A distributed control approach was designed by Zou and Meng (8) by introducing

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distributed estimators to obtain reference information for leader-follower control. Another distributed control algorithm was proposed by Dong et al. (9) to track the flight formation of multiple robot leader-follower. In addition, a non-smooth distributed control algorithm was developed by Du et al. (10), so that the robot leaderfollower control tracking was achieved. In addition, with the help of a sub-optimal  $H\infty$  strategy, a distributed leader-follower control algorithm is designed by Jasim et al. (11) that is robust to disturbances and parameter uncertainties. Although the control schemes proposed in the mentioned papers are convincing in hierarchical leader-follower formation control tracking, the control command extraction may cause singularities and chattering, which may cause implementation problems in practical applications. Also, in these articles, the flight group has a flight arrangement in a simple route, and the issue of moving target tracking has not been investigated. In this article, the MPC method is used for formation control in which there is no possibility of chattering, and the flight path is a spiral path, and the issue of moving target tracking is also investigated.

It is essential, to maintain the safety of the operations in the missions that the UAV group performs. One of the most important safety issues is avoiding obstacles. If a group of quadrotors encounters obstacles in an unknown environment, each drone must recognize the obstacle and pass through it. Crossing obstacles is necessary to avoid accidents and make the flight safe. This article focuses on the crossing of the quadrotor group through static and obstacles and maintaining the flight dynamic arrangement after crossing the obstacles. The methods of solving the collision avoidance problem are different for dynamic and static obstacles. A\* (12), Genetic (13), Differential Evolution (14), Ant Colony Optimization (15), and Particle Swarm Optimization (16) methods are usually used to avoid static obstacles. Methods for dealing with dynamic obstacles include Fuzzy Logic Algorithm (17), Neural Network (18), Rapidly-exploring Random Trees (19), and APF (20). Shang et al. (21) used the terminal nonsingular sliding mode controller for the problem of control formation and obstacle avoidance. Quadrotors have maintained formation flight after crossing obstacles. In this paper, only static obstacles are considered.

One of the most widely used methods to identify and avoid obstacles is the APF method. Which is expressed by mathematical equations and has advantages such as high safety and simplicity of calculations. In this method, a positive potential field is considered for obstacles, and a negative potential field for the target. The drone is attracted to the target by avoiding obstacles. Pan et al. (22) introduced formation control which is based on the leader-follower method, in which the PD is used to control the position and attitude of the quadrotors, and the APF is used to pass the obstacles. To prove the effectiveness of the above method, several experiments have been performed. In this article, crossing dynamic obstacles is not investigated. Wang and Zhang (23) have presented a rapidly-exploring random trees algorithm for the formation control and crossing obstacles, in which the lack of vigilance and low speed of the APF method is compensated by the sampling method. In this article, crossing static obstacles is considered. Qiao et al. (24) have provided formation control based on distributed control. The potential function is used to avoid the collision. A virtual navigator determines the movement of agents. In this article, the obstacles are static, and the drones maintain the connection after crossing. Aljassani et al. (25) presented a new APF method for the UAV group to pass through obstacles, which solves the problem of getting stuck in a local minimum. The leaderfollower method is used for group movement. The obstacles considered are two static obstacles. In these articles, the crossing of dynamic obstacles is not investigated. Huang et al. (26) have investigated dynamic obstacles avoidance and maintaining continuity and formation flight after crossing obstacles. The sliding mode method and the virtual potential field method are used for control formation and obstacle avoidance. Zhang et al. (27) proposed a distributed control method for quadrotor group flight formation. The disadvantages of this method are getting stuck in a local minimum and unreachable goals in environments full of obstacles (28). To solve these problems, some approaches have been proposed. Methods are also proposed for broader problems, such as dynamic obstacle avoidance or integration of UAV kinematic models to improve tracking accuracy (29, 30). In the mentioned articles, simultaneously crossing the dynamic and static obstacles and maintaining the flight formation after crossing the obstacles and tracking the mobility target simultaneously have not been discussed and, in a small number of these articles, the improvement of the potential field method has been investigated to solve its problems.

The necessity of doing this article is to improve the potential field method for the passage of the flight group through dynamic obstacles and maintain the connection between the agents.

The innovation of this paper is that it presented an improved potential field method for crossing static and dynamic obstacles and maintaining continuity after crossing obstacles. Where instead of considering a circular repulsion field for obstacles, an elliptical field is considered, which causes the repulsion range of obstacles to be greater and, as a result, solves the problem of getting stuck in the local minimum and not reaching the target in obstacle-filled environments to a great extent, and simultaneously, the leader tracks the moving target while maintaining the flight formation.

The article's structure is as follows: In the first section, the dynamic modeling of the quadrotor is

presented. The following section deals with attitude and position controllers. In the third section, the control formation is given; in the fourth section, the crossing of obstacles is discussed; and in the last section, the results are presented.

#### 2. DYNAMIC MODEL OF QUADROTOR

The six degrees of freedom model is obtained according to the Newton-Euler method. Total rotors velocity and the rotor velocity vector are as follows:

$$\Pi == + \varpi_4 + \varpi_2 - \varpi_1 - \varpi_3 \quad , \quad \Pi = \begin{bmatrix} \omega_1 \\ \varpi_2 \\ \varpi_3 \\ \varpi_4 \end{bmatrix}$$
(1)

where  $(\varpi_1, \varpi_2, \varpi_3, \varpi_4)$  show the speeds of the rotors. The effect of the motion vector on the quadrotor dynamics is given below:

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$$U_{B}(\varpi) = E_{B}\varpi^{2} = \begin{bmatrix} 0\\0\\U_{1}\\U_{2}\\U_{3}\\U_{4} \end{bmatrix} = \begin{bmatrix} 0\\0\\b(\varpi_{1}^{2} + \varpi_{2}^{2} + \varpi_{3}^{2} + \varpi_{4}^{2})\\b(\varpi_{4}^{2} - \varpi_{2}^{2})\\bl(\varpi_{3}^{2} - \varpi_{1}^{2})\\c_{d}(\varpi_{2}^{2} + \varpi_{4}^{2} - \varpi_{1}^{2} - \varpi_{3}^{2}) \end{bmatrix}$$
(2)

where, *l* is the length from the center of mass to each rotor,  $c_T$  is the thrust force coefficient, and  $c_d$  is the drag force coefficient. The  $E_B$  and  $U_B(\varpi)$ , which show the motion matrix and the motion vector, are as follows.

$$E_B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ c_T & c_T & c_T & c_T \\ 0 & -c_T l & 0 & c_T l \\ -c_T l & 0 & c_T l & 0 \\ -c_d & c_d & -c_d & c_d \end{bmatrix}$$
(3)

The dynamical equations of the quadrotor are given below:

$$\begin{split} \dot{\vartheta}_{1} &= \dot{\phi} = \ddot{\phi} + \ddot{\theta}sin\phi tan\theta + \ddot{\psi}cos \ \phi tan\theta \\ \dot{\vartheta}_{2} &= \dot{\theta} = \ddot{\theta}cos\phi - \ddot{\psi}sin \ \phi \\ \dot{\vartheta}_{3} &= \dot{\psi} = \frac{sin\phi}{cos\theta} \ddot{\theta} + \frac{cos\phi}{cos\theta} \ddot{\psi} \\ \dot{\vartheta}_{4} &= \dot{x} = \vartheta \\ \dot{\vartheta}_{5} &= \dot{y} = \vartheta \\ \dot{\vartheta}_{6} &= \dot{z} = \vartheta \\ \dot{\vartheta}_{7} &= \dot{P} = \frac{I_{YY} - I_{ZZ}}{I_{XX}} RQ - \frac{J_{TP}}{I_{XX}} Q \ \Omega + \frac{U_{2}}{I_{XX}} \\ \dot{\vartheta}_{8} &= \dot{Q} = \frac{I_{ZZ} - I_{XX}}{I_{YY}} RP + \frac{J_{TP}}{I_{YY}} P \ \Omega + \frac{U_{3}}{I_{YY}} \\ \dot{\vartheta}_{9} &= \dot{R} = \frac{I_{XX} - I_{YY}}{I_{ZZ}} PQ + \frac{U_{4}}{I_{ZZ}} \end{split}$$

$$\begin{split} \dot{\vartheta}_{10} &= \dot{U} = (-WQ + VR) + gs_{\theta} \\ \dot{\vartheta}_{11} &= \dot{V} = (-UR + WP) - gc_{\theta}s_{\phi} \\ \dot{\vartheta}_{12} &= \dot{W} = (-UQ + VP) - gc_{\theta}s_{\phi} + \frac{U_{1}}{m} \end{split}$$
(4)

where,  $J_{Tp}$  is the moment of total rotation of inertia about the rotor axis, (U, V, W) are the linear velocities, (P, Q, R) are roll, pitch, and yaw, and  $I_{XX}$ ,  $I_{YY}$ , and  $I_{ZZ}$  are the moments of inertia in the x, y, and z-axis, whose values are given in Table 1. the rotors speed inputs  $U_1, U_2, U_3$ , and  $U_4$  are as follows (21):

$$U_{1} = c_{T}(\varpi_{1}^{2} + \varpi_{2}^{2} + \varpi_{3}^{2} + \varpi_{4}^{2})$$

$$U_{2} = lc_{T}(-\varpi_{2}^{2} + \varpi_{4}^{2})$$

$$U_{3} = lc_{T}(-\varpi_{1}^{2} + \varpi_{3}^{2})$$

$$U_{4} = c_{d}(-\varpi_{1}^{2} + \varpi_{2}^{2} - \varpi_{3}^{2} + \varpi_{4}^{2})$$

$$\varpi = -\varpi_{1} + \varpi_{2} - \varpi_{3} + \varpi_{4}$$
(5)

#### **3. MPC CONTROLLER**

The predictive controller is used in the industry because of its advantages, such as dealing with disturbances, limitations and uncertainties. In this article, a generalized predictive controller is used, which has features such as dealing with non-minimum phase systems and having additional control horizon parameters. In this controller, the control signal is obtained by minimizing the multistep function in the prediction horizon. As a result, according to the integral behavior in the state space, it is possible to replace u(k) with  $\Delta u(k) = u(k) - u(k -$ 1) in the equations. The state space equations are given below:

$$\begin{bmatrix} \Delta x_m(k+1) \\ y(k+1) \end{bmatrix} = \begin{bmatrix} A_m & 0^T_{q \times n} \\ C_m A_m & I_{q \times q} \end{bmatrix} \begin{bmatrix} \Delta x_m(k) \\ y(k) \end{bmatrix} + \begin{bmatrix} B_m \\ C_m B_m \end{bmatrix} \Delta u_m(k) + \begin{bmatrix} B_d \\ C_m B_m \end{bmatrix} \varepsilon(k)$$
(6)  
 
$$y(k) = \begin{bmatrix} 0^T_{q \times n} & I_{q \times q} \end{bmatrix} \begin{bmatrix} \Delta x_m(k) \\ y(k) \end{bmatrix}$$

**TABLE 1.** Parameters of quadrotor dynamic

Parameter	Value
I <sub>XX</sub>	$11  imes 10^{-2} \ kg \ m^2$
$I_{YY}$	$19  imes 10^{-2} \ kg \ m^2$
I <sub>ZZ</sub>	$1.3 imes10^{-2}~kg~m^2$
$J_{Tp}$	$6  imes 10^{-5} kg m^2$
т	3.23 kg
l	0.23 m
C <sub>d</sub>	$7.5  imes 10^{-7} Nm s^2$
c <sub>T</sub>	$3.13 \times 10^{-5} N s^2$

The output is defined as below:

$$Y = H'x(k) + H".\Delta U \tag{7}$$

where:

$$H' = \begin{bmatrix} CA \\ CA^{2} \\ CA^{3} \\ \vdots \\ CA^{N_{p}} \end{bmatrix}, H'' = \begin{bmatrix} CB & 0 & 0 & \dots & 0 \\ CAB & CA & 0 & \dots & 0 \\ CA^{2}B & CAB & CB & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ CA^{N_{p}-1}B & CA^{N_{p}-2}B & CA^{N_{p}-3}B & \dots & CA^{N_{p}-N_{c}}B \end{bmatrix}$$
(8)

The cost function is considered as below:

$$J = (Y - w)^T W_y (Y - w) + \Delta U^T W_u \Delta U$$
(9)

where, Y is the vector of predicted outputs, w is the vector of reference signal values in future times,  $\Delta U$  is the control signal, and  $W_u$  and  $W_y$  define the weight of inputs and outputs in the cost function.

The necessary condition for minimizing the cost function is given below:

$$\frac{\partial f}{\partial A H} = 0$$

By satisfying the above condition, u is obtained as follows (31):

$$\Delta U = (H^{"T}W_{y}H^{"} + W_{u})^{-1}H^{"T}W_{y}(w - H'x(k))$$
(10)

#### **4. FORMATION FLIGHT**

Formation control patterns include virtual structure and behavior-based, and leader-follower. In the virtual structure method, each agent is considered an element of a larger structure. In this method, all the arrangement members act as a single rigid body and follow a determined path. This method is suggested to maintain formation while moving. As a result, this method is unsuitable for crossing a group of obstacles because it is necessary to change the formation to pass the obstacles. In addition to the group movement, searching and reaching the desired target is also investigated in the behavior-based structure. The weakness of this method is the difficulty of analyzing the overall behavior of the formation and its mathematical analysis and checking its stability.

In the leader-follower algorithm, one or more agents are designated as leaders, and other quadrotors are considered followers, so the followers must follow the leader with a fixed direction and position. The control of the formation of multi-agent systems using the leaderfollower structure has received special attention due to its simplicity and scalability. Since the movement of other vehicles in the formation is completely determined by the leading position, the leading position creates coordination. Therefore, the followers follow the leader to maintain the formation. The advantage of this method is that it is easy to understand and more practical in implementation. This model is used in this article.

**4. 1. Formation Control** In this article, quadrotor group control formation and obstacle avoidance are investigated. Formation flight is controlled by the MPC method. The pattern used is leader-follower. In the leader-follower method, the leader follows a determined path, and the followers maintain a certain angle and distance from the leader. Figure 1 illustrates this method. In this figure,  $\lambda$  is the distance from the center of the leader mass to the center of the follower mass, and  $\varphi$  is the angle between the x-axis and  $\lambda$  line.

$$\begin{cases} \lambda_x = -(x_L - x_F) \cos \psi_L - (y_L - y_F) \sin \psi_L \\ \lambda_y = -(x_L - x_F) \sin \psi_L - (y_L - y_F) \cos \psi_L \end{cases}$$
(11)

$$\lambda_x^d = \lambda \cos \varphi$$

$$\lambda_y^d = \lambda \sin \varphi$$
(12)

The formation error is given below:

$$\begin{cases} e_x = \lambda_x^d - \lambda_x \\ e_y = \lambda_y^d - \lambda_y \\ e_\psi = \psi_F - \psi_L \end{cases}$$

$$\begin{cases} \dot{e}_x = \dot{\lambda}_x^d - \dot{\lambda}_x \\ \dot{e}_y = \dot{\lambda}_y^d - \dot{\lambda}_y \\ \dot{e}_\psi = \dot{\psi}_F - \dot{\psi}_L \end{cases}$$
(13)

 $\lambda^d$  and  $\varphi^d$  are constant parameters, therefore,  $\lambda_x^d$  and  $\lambda_y^d$  have constant values and, their derivatives  $\dot{\lambda}_x^d$  and  $\dot{\lambda}_y^d$  are zero. The transition dynamics on the x-y plane are present below:

$$\begin{cases} \dot{x}_i = v_{ix} \cos \psi_i - v_{iy} \sin \psi_i \\ \dot{y}_i = v_{ix} \sin \psi_i + v_{iy} \cos \psi_i \\ \dot{\psi}_L = \omega_L \end{cases}$$
(14)



Figure 1. Quadrotor formation in x-y plane

i indicate leader (i = L) or follower (i = F).  $\dot{x}_i$  and  $\dot{y}_i$  are velocities in the ground coordinate system.  $\psi_i$  is the angle between the x-axis of the body and the ground coordinate system, and  $v_{ix}$  and  $v_{iy}$  are the velocities in the body coordinate system:

$$\begin{cases} v_{ix} = \dot{x}_i \cos \psi_i + \dot{y}_i \sin \psi_i \\ v_{iy} = -\dot{x}_i \sin \psi_i + \dot{y}_i \cos \psi_i \end{cases}$$
(15)

As a result, the following relations are obtained.

$$\begin{cases} \dot{e}_x = -(\lambda_y^d - e_y)\omega_L - v_{Fx}\cos e_{\psi} + v_{Fy}\sin e_{\psi} + v_{Lx} \\ \dot{e}_y = (\lambda_x^d - e_x)\omega_L - v_{Fx}\sin e_{\psi} - v_{Fy}\cos e_{\psi} + v_{Ly} \\ \dot{e}_{\psi} = \omega_F - \omega_L \end{cases}$$
(16)

The state space is as below.

$$\dot{x} = A(x) + B(x)\tau \tag{17}$$

where x is the state vector and  $\tau$  is the control input, and M(x) and N(x) are defined as follows (32):

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{e}_{\boldsymbol{x}} & \boldsymbol{e}_{\boldsymbol{y}} & \boldsymbol{e}_{\boldsymbol{\psi}} \end{bmatrix}^T \tag{18}$$

$$\tau = \begin{bmatrix} \tau_{Fx} & \tau_{Fy} & \omega_F \end{bmatrix}^T \tag{19}$$

$$A(x) = \begin{bmatrix} e_y \omega_L + \tau_{Lx} - \omega_L \lambda_y^d \\ -e_x \omega_L + \tau_{Ly} + \omega_L \lambda_x^d \\ -\omega_L \end{bmatrix}$$
(20)

$$B(x) = \begin{bmatrix} -\cos e_{\psi} & \sin e_{\psi} & 0\\ -\sin e_{\psi} & -\cos e_{\psi} & 0\\ 0 & 0 & 1 \end{bmatrix}$$
(21)

The control law for the formation of the quadrotors based on MPC (33) is considered as follows:

$$\begin{split} M_{i}(k) &= -\sum_{j=1}^{N+1} a_{ij} \left[ \sum_{k=0}^{3} \beta_{k} \left( f_{i}^{(k)} - \hat{f}_{j}^{(k)} \right) \right], \\ i \in \{1, 2, \dots, N\}, \\ \hat{f}_{j}^{(k)} &= f_{j}^{(k)} - d_{fj}^{(k)}, \ j \in \{1, 2, \dots, N+1\}, \\ \begin{cases} \beta > 0 \ \forall k \in \{0, 1, 2, 3\} \\ \lambda_{min} > \frac{\beta_{1}^{2}}{\beta_{1} \beta_{2} \beta_{3} - \beta_{0} \beta_{3}^{2}} \\ \beta_{1} \beta_{2} > \beta_{0} \beta_{3} \end{cases} \end{split}$$
(22)

where *i* and *N* + 1 represent quadrotor *i* and the leader. The control gains  $\beta_k \epsilon \mathbb{R}$ ,  $k \epsilon \{0, 1, 2, 3\}$  must satisfy conditions (13).  $d_{fj}^{(k)} \epsilon \mathbb{R}^2$  is the desired state between *quadrotor j* and the leader on the horizontal plane. The control law for the formation flight of *quadrotor i* in the vertical direction (34) is as follows:

$$T_{i}(k) = -\sum_{j=1}^{N+1} a_{ij} \left[ \sum_{k=0}^{3} \gamma_{k} \left( h_{i}^{(k)} - \hat{h}_{j}^{(k)} \right) \right],$$
  

$$i \in \{1, 2, \dots, N\},$$
  

$$\hat{h}_{j}^{(k)} = h_{j}^{(k)} - d_{hj}^{(k)}, \quad j \in \{1, 2, \dots, N+1\},$$
  

$$k \in \{0, 1\},$$
  
(23)

$$\gamma_k > 0, \ k \in \{0, 1\},$$

where  $\gamma_k \in \mathbb{R}$   $k \in \{0, 1\}$  is control gains and  $d_{hj}^{(k)} \in \mathbb{R}^2$  is the desired relative state between *quadrotor j* and the leader in the vertical direction.

#### **5. IMPROVED ARTIFICIAL POTENITIAL FIELD**

In the APF, attractive potential is considered for the target, and repulsive potential is considered for the obstacles. The agent moves away from the obstacles by moving towards the target.

The control of the agent by the AFP is as below:

$$U_{ar}(x) = U_a(x) + U_r(x)$$
 (24)

where,  $U_{ar}$ ,  $U_a$ , and  $U_r$ , represent the potential of attraction, the potential of repulsion, and the potential virtual field. Gradient functions are stated as follows:

$$F_{art} = F_a + F_r$$

$$F_a = -grad[U_a(x)]$$

$$F_r = -grad[U_r(x)]$$
(25)

where  $F_a$  is the robot's attraction, and  $F_r$  is the force created by  $U_r(x)$ . The attraction coefficient  $k_a$  and the potential attraction field  $U_a(x)$  are given below:

$$U_a = \frac{1}{2}k_a R_a^2 \tag{26}$$

The  $U_r$  (x) is as follows:

$$U_r(x) = \begin{cases} 0.5k_a(\frac{1}{R_r} - \frac{1}{X_0})^2 & R_r \le X_0\\ 0 & R_r > X \end{cases}$$
(27)

where  $X_0$  is the safe distance from the obstacles.

 $\frac{R_a = ||X_d - X|| =}{\sqrt{(x - x_d)^2 - (z - z_d)^2 - (y - y_d)^2}}$  is the distance from the agent to the target,  $R_r = ||X_u - X|| =$  $\sqrt{-(z - z_u)^2 + (x - x_u)^2 - (y - y_u)^2}$  is the shortest distance from the agent, and the obstacles, where X = $(x, y, z), X_m = (x_m, y_m, z_m)$ , and  $X_d = (x_d, y_d, z_d)$  are the position of the agent, the position of obstacles and the position of the target. The functions of repulsion and attraction are present below:

$$F_{a} = -\nabla \left(\frac{1}{2}k_{a}R_{a}^{2}\right)k_{a}R_{a}$$

$$U_{r}(x) = \begin{cases} k_{a}(\frac{1}{R_{r}} - \frac{1}{R_{r}^{2}})\frac{1}{R_{r}^{2}} & R_{r} \leq X_{0} \\ 0 & R_{r} > X_{0} \end{cases}$$
(28)

The traditional APF method works poorly in obstacle environments, and may get stuck in a local minimum. To solve this issue, the improved APF is used. The spherical repulsion field has been changed to an elliptic field in the APF. According to Figure 2, the agent is placed in the center of the ellipse and the locations of the obstacles are C and D. Around the agent, there is an ellipse repulsion field, and the obstacles are placed on the edges of the ellipse, which have different distances from the agent. As a result, the repulsive field created can repel obstacles more effectively (The range of repulsive increases). The advantage of this way is that it allows a greater safety distance for the agent to pass and makes it easier to pass obstacles in complex environments. The parameters of the ellipsoidal APF are proportional to the velocity of the agent. The magnitudes of its long semi-axis  $\boldsymbol{a}$  and middle semi-axis  $\boldsymbol{b}$  are determined by the components of the agent's velocity. The focal length is  $c_1 = \sqrt{\alpha^2 - \beta^2}$ , and combined with the agent's coordinates and the velocity direction can be derived from the coordinates of the two focal points of the ellipse, as follows:

$$x_{c1} - x_m = -\varrho v_x$$
  

$$y_{c1} - y_m = -\varrho v_y$$
  

$$z_{c1} - z_m = -\varrho v_z$$
  

$$(x_{c1} - x_m)^2 + (y_{c1} - y_m)^2 + (z_{c1} - z_m)^2 = a^2 - \beta^2$$
  

$$x_{c2} - x_m = -\varrho v_x$$
  

$$y_{c2} - y_m = -\varrho v_y$$
  

$$z_{c2} - z_m = -\varrho v_z$$
  

$$(x_{c2} - x_m)^2 + (y_{c2} - y_m)^2 + (z_{c2} - z_m)^2 = a^2 - \beta^2$$
  
(29)

where  $(x_m, y_m, z_m)$ ,  $(x_{H1}, y_{H1}, z_{H1})$ , and  $(x_{H2}, y_{H2}, z_{H2})$  are the coordinates of the robot and focal  $H_1, H_2$  of the ellipse. The condition for determining the presence of obstacles in the improved APF requires the geometric definition of an ellipse and the sum of the distances from the obstacles to the two focal points of the ellipse are:

$$d^{1}, A, H_{1}, H_{2} = \sqrt{(x - x_{H1})^{2} + (y - y_{H1})^{2} + (z - z_{H1})^{2}} + \sqrt{(x - x_{H2})^{2} + (y - y_{H2})^{2} + (z - z_{H2})^{2}}$$
(30)

The mentioned equation can be approximated as follows:

$$d, A, H_1, H_2 = d^1, A, H_1, H_2 - 2X_0$$
(31)



Figure 2. Diagram of the APF with elliptical cross-section

If  $A, H_1, H_2 \leq 2\alpha$  The obstacle will probably collide with the agent and needs a way to avoid the collision. If  $A, H_1, H_2 > 2\alpha$  there is no possibility of collision. For ease of calculations, the repulsive function of the improved APF is considered as below:

$$U_{r} = \begin{cases} \frac{1}{2} k_{\alpha} \left( \frac{1}{d_{A,H_{1},H_{2}-2\alpha}} - \frac{1}{x_{0}} \right),^{2} & A, H_{1}, H_{2} \leq \\ 0, & A, H_{1}, H_{2} > 2\alpha \end{cases}$$
(32)  
2 $\alpha$ 

The repulsive force on the agent is given below:

$$F_{r} = -\Delta U_{r} = \begin{cases} k_{a} \left( \frac{1}{d,A,H_{1},H_{2}-2\alpha} - \frac{1}{X_{0}} \right) \frac{1}{d^{2}A,H_{1},H_{2}}, d \quad A,H_{1},H_{2} \le 2\alpha \\ 0, \qquad A,H_{1},H_{2} > 2\alpha \end{cases}$$
(33)

where  $dx, x_{H1}, x_{H1} \le 2\alpha$  indicates the repulsive force that acts within the ellipsoid. The total force on the agent is as below:

$$F_{total}(x) = \sqrt{(F_{ax} + F_{rx})^2 + (F_{ay} + F_{ry})^2 + (F_{az} + F_{rz})^2}$$
(34)

#### **5. SIMULATIONS AND RESULTS**

In this section, the results of obstacle avoidance using the improved APF for a group of quadrotors (Figure 3) in 4 missions are present. First, the simulation results of quadrotor attitude and position control are presented by the MPC method.

Figure 4 shows the attitude of the quadrotor controlled using the MPC method. Severe overshoot and undershoot are not seen in the responses. The convergence time of  $(\phi, \theta, \psi)$  are (1,0.9,2) seconds.

Figure 5 shows the position of the robot. According to this figure, the responses track the reference well and converge in less than 1 second.

In the following, the simulation results of the control formation are presented.

Figure 6 indicates the position of robots in the S-shaped path in which five follower quadrotors follow the leader.

Figure 7 indicates the attitude of quadrotors in the S-shaped path in which five follower quadrotors follow the leader well. The maximum convergence time of the follower's attitude ( $\phi, \theta, \psi$ ) is (6s,6s,9s).

Figure 8 presents the position of agents in 3D space, where followers follow the leader in the S-shaped path.

The results of the formation flight simulation are more than 90% consistent with the reported data in literature (32, 35).

The results of avoiding collision with obstacles using the improved APF are given in 3 missions. In the first mission, the quadrotors have a square formation that



Figure 3. Formation control block diagram



Figure 4. Response curves of attitude for quadrotor



Figure 5. Response curves of position for quadrotor



Figure 6. The position of the robots in the S-shaped path



Figure 7. The attitude of the quadrotors in the s-shaped path



Figure 8. 3D diagram of quadrotors along the s-shaped path

passes through static obstacles. In the second mission, the quadrotors have a square arrangement, and the obstacles are dynamic. In the third mission, the quadrotors have a hexagonal arrangement, and the obstacles are fixed. In this mission, the target is dynamic. In the final mission, the quadrotors have a hexagonal arrangement, and the obstacles are dynamic.

The results of the first mission are given in Figure 9. The quadrotors have passed the static obstacles and have maintained a square formation, and the leader has reached the target. In this figure, the leader is at the point (-3, -43), and after passing the obstacles, she reaches the point (7, 20). Followers are also located at points (-10, 50), (-3, 50) and (-10, -43), and after passing the dynamic obstacles, they are placed in points (-3, 10), (7, 9.5), and (-3, 19.5), which maintain up to 95% accuracy of the square shape after passing the obstacles. The locations of obstacles are shown in Table 2.

In the second mission, four agents were considered. The obstacles are dynamic. The simulation results of this mission are given in Figures 10-12. The velocity of all obstacles is V = [-3t(i), 9t(i), 12t(i)].



Figure 9. The flight path of the agents in the square arrangement

<b>TABLE 2.</b> Position of obstacles					
Obstacle	X(m)	Y(m)	Z(m)		
1	-10	-40	15		
2	-10	-35	14		
3	-10	-30	12		
4	-10	-20	15		
5	-10	-10	12		
6	-10	-5	12		
7	-10	0	15		
8	-15	0	20		
9	-20	0	20		
10	-20	-5	18		
11	0	-40	25		
12	0	-35	15		
13	0	-30	15		
14	0	-20	20		
15	0	-10	20		
16	0	0	18		
17	5	0	18		
18	10	0	15		
19	15	0	15		
20	20	0	20		



Figure 10. The positions of the agents at the beginning of the flight

Figure 10 indicates the position of the agents at the beginning of the flight, as well as the expected position of the agents after crossing the obstacles.

Figure 11 presents the position of agents while crossing the obstacles.

Figure 12 indicates the position of agents after crossing the obstacles. This figure shows the successful

passing of the agents through the dynamic obstacles and maintaining the square arrangement after crossing. As it is clear from Figures 10, 11, and 12, the leader is at the point (-3, -43) at the beginning of the flight, and after passing the dynamic obstacles, it reaches the point (10, 30). Which is as expected. Followers, who were initially located at points (-10, -50), (-3,50), and (-10, -43), after passing the obstacles, reach points (3, 19.7), (10, 20) and (3, 29.6), which as expected should be at points (3, 20), (10, 20) and (3, 30), and therefore, the simulation with 95% accuracy has kept its square formation and is as expected.

In the third mission, the number of agents has increased to 6. Obstacles are fixed, and the target is moving. The simulations of this mission are presented in Figure 13. The results indicate that the quadrotors passed the obstacles, and the leader tracked the target. According to Figure 13, the leader is at point (40, 32) at the beginning of the flight, and after passing through the obstacles, it reaches point (129, 107), which is expected to reach point (130, 107). Also, the followers are located at points (40, 15), (30, 15), (22, 22), (30, 32), and (47, 22)



Figure 11. Agents crossing obstacles during flight



Figure 12. The position of the agents after crossing the obstacles



at beginning of the flight, which reach points (130, 90), (120, 91), (112, 98), (120, 107) and (140, 98) after passing the static obstacles. Which, as expected, should be placed in points (130, 90), (120, 90), (112, 97), (120, 107), and (140, 97), respectively. Therefore, the simulations maintain the hexagonal formation with an accuracy of more than 95%. Also, in this mission, the target is moving and is first located at the point (90, 65) and reaches the point (120, 107), which the leader tracks. The location of the obstacles is shown in Table 3.

In the fourth mission, six robots are considered. Obstacles are dynamic, and the target is static. The simulations of this mission are present in Figures 14-16. Figure 14, shows the initial position of the quadrotors and target.

TABLE 3. O	bstacles position
------------	-------------------

Obstacle	X(m)	Y(m)	Z(m)
1	50	5	20
2	50	10	20
3	50	15	20
4	50	16	20
5	50	16	20
6	50	50	22.5
7	50	55	22.5
8	50	60	22.5
9	50	65	22.5
10	50	70	22.5
11	50	75	22.5
12	60	40	22.5
13	50	20	20
14	60	50	22.5
15	60	60	22.5



Figure 14. The initial position of quadrotors, obstacles, and targets

Figure 15 indicates that the quadrotors are crossing obstacles, and the leader is moving towards the target.

Figure 16 indicates the quadrotors passing through the moving obstacles and the leader reaching the target. After passing through the obstacles, the quadrotors preserve the hexagonal flight arrangement.

In these figures, it is clear that the leader is initially located at point (40, 40) and reaches point (90, 71) after passing the obstacles. As expected, it should reach the point (90, 70). Other followers are located at the points (40, 20), (30, 20), (20, 30), (30, 40), and (47, 30) at the beginning of the flight, and after passing the dynamic obstacles, they have reached the points (90, 51), (80, 49), (70, 59), (80, 71) and (97, 60) according to Expectations should have reached the points (90, 50), (80, 50), (70, 60), (80, 70) and (97, 60). These results showed that the flight group maintained the hexagonal flight arrangement after crossing the obstacles with 95% accuracy. These results are consistent with crossing the obstacles of



Figure 15. Agents passing through dynamic obstacles



Figure 16. Preserving formation flight after crossing obstacles

reported in literature (36), in which the APF method was used.

In this section, the simulation results are given. First, the results of controlling the position and condition of the quadrotor are shown. The quadrotors converged to the reference in less than two seconds, and there was no sharp fluctuation in the responses. The results of formation control show that five quadrotors have followed the leader. Finally, the results of avoiding collisions with obstacles on the improved artificial potential field in four missions were presented. In the first mission, four quadrotors were considered, and the obstacles were static. In the second mission, four agents crossed dynamic obstacles. In the third mission, six quadrotors crossed static obstacles, and the target was moving. In the last scenario, six quadrotors crossed dynamic obstacles. The results of these simulations showed that the quadrotors maintained their flight formation after crossing the obstacles with 95% accuracy.

#### 6. CONCLUSION

In this article, quadrotor formation control and obstacle avoidance, and moving target tracking are investigated. To achieve this goal, in the first step, the simulations of the position and attitude controller were presented, which showed that the convergence time of the responses is at most 3 seconds, which is an acceptable time, and severe overshoot and undershoot were not observed. The results of simulation of formation control by the MPC method in an S-shaped path and linear arrangement show that the followers follow the leader and maintain a certain distance and angle from the leader. Obstacle-crossing results using the improved APF were presented in 4 missions. In the first scenario, three quadrotors followed the leader and crossed static obstacles, and maintained a square formation. In the second scenario, four quadrotors passed dynamic obstacles and, after passing and preserved the square formation. In the third mission, six quadrotors crossed the static obstacles, and the leader tracked the moving target. In the last mission, six quadrotors crossed the dynamic obstacles. In these two missions, the flight group maintained a hexagonal formation after passing through the dynamic and static obstacles. The results of these simulations show the success of the method used to track the moving target and pass the quadrotors through fixed and moving obstacles, by increasing the agents and changing the flight formation. Also, the problem of getting stuck in the local minimum and not passing through environments with many obstacles has not occurred, which indicates the efficiency of the improved APF method.

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#### Persian Abstract

#### چکیدہ

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هدف از این مقاله کنترل شکل دهی و عبور از موانع ایستا و دینامیک برای گروه کوادروتور، حفظ تداوم و آرایش پرواز پس از عبور از موانع و ردیابی هدف متحرک است. برای کنترل وضعیت و موقعیت کوادروتورها و کنترل شکل دهی از روش MPC استفاده شده است. شکل گیری پرواز بر اساس روش پیرو-پیشرو است که در آن پیروان با استفاده از کنترل کننده شکل دهی، زاویه و فاصله مشخصی را از پیشرو حفظ می کنند. روش APF بهبود یافته برای عبور از موانع استفاده شده است که مزیت اصلی آن در مقایسه با APF سنتی افزایش برد نیروی دافعه موانع است که مشکل گیر افتادن در حداقل محلی و عدم عبور در محیطهای پرمانع را حل میکند. نتایج طراحی کنترل کننده وضعیت و موقعیت نشان داد که کوادروتورها در کمتر از سه ثانیه همگرا شدند. شبیه سازیهای کنترل شکل دهی در مسیر مارپیچی نشان داد که پیروان، از رهبر پیروی میکنند. نتایج عبور کوادروتورها از موانع در جهار ماموریت ارائه شد. در ماموریت اول چهار کوادروتور از موانع ساکن عبور کردند. در ماموریت دوم چهار کوادروتور از موانع دینامیکی عبور کردند. در این دو ماموریت، کوادروتورها از موانع ساین در ماموریت اول چهار کوادروتور از موانع سای عبور کردند. در این دوم جهار کوادروتور از موانع دینامیکی عبور کردند. در این دو ماموریت، کوادروتورها از موانع ساین عبور کردند. در ماموریت سوم تعداد کوادروتورها از موانع دینامیکی عبور متحرک را ردیابی کرد و کوادروتورها از موانع ساکن عبور کردند. در ماموریت سوم تعداد کوادروتورها از موانع دینامیکی عبور مودید. در این دو ماموریت، کوادروتورها از موانع ساکن عبور کردند. در آخرین ماموریت، کوادروتورها از موانع دینامیکی عبور مانور در این متحرک را ردیابی کرد و کوادروتورها از موانع ساکن عبور کردند. در آخرین ماموریت، کوادروتورها از موانع دینامیکی عبور کردند و لید هدف ثابت را ردیابی کرد. در این ماموریت ها، کوادروتورها از موانع ساکن عبور کردند. در آخرین ماموریت، کوادروتورها از موانع دینامیکی عبور کردند و لید هدف ثابت را دردیابی کرد. در این ماموریت ها، کوادروتورها از موانع آریش شان ضلعی را حفظ می کنند. شبیه سازی نتایج نشان داد که کوادروتورها از موانع ثابت و محرک عبور کرده و پس از مور، آرایش پرواز را حفظ کردند.



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# Corrosion Behavior Evaluation of Nanolayered CrN/CrAlN Coatings on Titanium and Ti6Al4V Substrates

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#### PAPER INFO

#### ABSTRACT

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Keywords: CrN/CrAIN Coating Titanium Ti6A14V PVD Ringer Solution Corrosion Behavior In recent years, implants are used as prostheses to replace and protect bone. Titanium, as an implantable material, needs to improve corrosion and wear properties for better performance. Therefore, in the current study nitride coatings were applied with the aim of improving corrosion and wear properties. Cathodic arc evaporation physical vapor deposition (CAE-PVD) technique was used to deposit nanolayered CrN/CrAIN coatings on commercially pure titanium and Ti6Al4V substrates for biomaterial applications. X-ray diffraction (XRD) was used to characterize the crystal structure of the coating, and scanning electron microscopy (SEM) and field emission scanning electron microscopy (FESEM) were utilized to observe the surface morphology and cross-section of the coating. The coating adhesion was measured according to VDI 3198 standard using a Rockwell-C indenter. The corrosion behavior was evaluated by potentiodynamic polarization and spectroscope electrochemical impedance in Ringer's solution. The results showed that the nanolayered coating changed the corrosion potential from -0.368 V to -0.054 V for the titanium sample and from -0.405 V to -0.028 V for the Ti6Al4V specimen. Additionally, the corrosion current density was reduced to about one-eighth and a third for the titanium and Ti6Al4V coated samples, respectively. The capacitator circle diameters increased due to the deposition of CrN/CrAIN coating, demonstrating enhanced corrosion behavior of the coated samples compared to uncoated specimens, as the coating acted as a barrier against corrosive liquids accessing the substrate.

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#### **1. INTRODUCTION**

As an implant material, titanium has been widely used in various medical applications due to its excellent biocompatibility properties, including the spontaneous formation of a stable and dense oxide layer on its surface. Additionally, titanium and its alloys have favorable mechanical, physical, and biological properties for implantation (1, 2). The desired characteristics of titanium and its alloys include a relatively suitable elastic modulus, good formability and machineability, excellent biocompatibility, and superior corrosion resistance compared to stainless steel and cobalt base-alloys (3). Therefore, damaged tissues can be replaced by titanium and its alloys in various situations (1).

However, pure titanium and Ti6Al4V alloy have some drawbacks such as low wear resistance, the

possibility of passive layer interaction with H<sub>2</sub>O (4), weak shear strength, and difficult production technique. Moreover, the surface oxide layer creates high friction and intensified wear rate for these materials. When the protective coating breaks down, the titanium substrate gets exposed to the surrounding environment, and if the protective layer is not repaired, the titanium is strongly exposed to shear stresses which can result in the formation of cold sores between it and the surrounding joints. Alternative separation and reformation of the oxide layer on the titanium surface consume the implant material. By continuing this phenomenon, the surface roughness increases, hard and coarse particles are created, causing abrasive wear at the implant surface (5). The worn particles can cause blood clots and swelling of the surrounding regions, leading to implant replacement and serious patient suffering (6, 7). Additionally, the

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higher elastic modulus of this material compared to that of bone can cause the stress shielding phenomenon (8). Moreover, using Ti6Al4V alloy as a long-term implant can create problems due to potential releases of vanadium and aluminum ions which may cause cellular toxicity and tissue noxious reactions (6, 7). Therefore, improving the corrosion resistance of titanium implants is essential to increase their biocompatibility and prolong their life (9, 10).

Surface modification is a method to enhance the chemical, mechanical, and biomedical properties of titanium composition. It can be achieved by chemical or mechanical methods (11, 12), such as shot penning (13, 14), sol gel (15), chemical vapor deposition (16), plasmaassisted chemical vapor deposition (17), thermal sputtering (18), electrochemical plating (19, 20), and physical vapor deposition (21-23). Among the abovementioned techniques, cathodic arc evaporation, due to the creation of uniform properties such as continuous, dense, and homogeneous coating, high adhesion to the substrate, material structure protection, and the possibility of multilayer coating deposition, can be used to form nitride coatings. Nitride coatings have several desirable properties, including high chemical stability, favorite hardness and adhesion, excellent resistance to corrosion and wear, as well as good hammering (24).

Studies have shown that nitride coatings deposited on titanium and its alloys using cathodic arc evaporation can improve their corrosion resistance. Olia et al. (25) deposited CrN/CrAlN and TiN/TiAlN coatings on stainless steel using the cathodic arc evaporation method, and corrosion tests in 3.5% NaCl solution showed that Ecoor of coated samples shifted to more positive potential. Khan et al. (26) also coated stainless steel using TiN, CrN, AlTiN, and AlCrN and evaluated their electrochemical behaviors. The coated samples had better corrosion resistance, with the CrN coating showing the best corrosion resistance. Additionally, different nitride coatings were deposited on steel substrates using cathodic arc evaporation, and the corrosion behavior was evaluated in 0.1M Na<sub>2</sub>SO<sub>4</sub> and 0.1M NaCl environments (27). The Ti-based coatings exhibited the best corrosion resistance and surface properties.

Several studies have been performed within the field of CrAlN coatings research (16, 28). The distinctive aspect of this study, in comparison to previous research, involves the utilization of two distinct substrates, including pure Ti and Ti6Al4V, and the subsequent evaluation of their respective corrosion characteristics in relation to one another. To enhance the performance of titanium as an implantable material, it is imperative to address the concerns regarding its corrosion and wear properties. Hence, in the present investigation, nitride coatings were employed with the objective of enhancing the corrosion resistance and wear characteristics. Therefore, the aim of this investigation is to study and assess the corrosion behavior of CrN/CrAlN coating deposited using cathodic arc evaporation on titanium and Ti6Al4V substrates in the Ringer solution.

#### 2. MATERIALS AND METHODS

#### 2.1. Surface Preparation and Coating Parameters

To achieve a high-quality and desired surface for coating, pure commercial titanium and Ti6Al4V alloy samples were prepared in sheet form and polished using 120 to 3000 grit sandpapers. Following this, the samples were washed in an acetone solution using an ultrasound device for ten minutes. Finally, CrN/CrAIN nano-coatings were deposited on the titanium and Ti6Al4V substrate using the cathodic arc evaporation method. The coating parameters are briefly summarized in Table 1.

2. 2. Coating Characterization The X-ray diffraction device (1730 PW Philips and PANalytical) was used to identify the structures and types of coating phases formed. The angle diffraction was selected in the range of 10-80 degrees with a step size of 0.05 degrees. To observe the cross-section of the coating, the titanium sample was first cut with a guillotine and then prepared for photography after the mount treatment, sanding, and polishing. A gold coating was applied to make the mount conductive. The surface morphology and cross-section of the coating were observed using scanning electron microscopy (840A-JSM, Jeol) and field emission scanning electron microscopy (Czech, TESCAN, MIRA3, FESEM), and the energy distribution spectrum was obtained by SAMX, France. The surface roughness was measured using a roughness meter (Roughness Tester PCE RT 2200). The adhesion test was carried out by applying 150 N force for 25 seconds using a Rockwell-C indenter and VDI3198 standard. The impression created by the indenter was observed via optical microscopy. According to the VDI3198 standard, coatings having adhesion conditions HF1 to HF3 are acceptable, whereas HF4 to HF6 states could be rejected. The classification of coating adhesion based on the VDI3198 standard is illustrated in Figure 1.

**TABLE 1.** The coating process parameters used in the present work

WOIK	
Working pressure (torr)	$5  imes 10^{-3}$
Target electrical current (A)	100
Substrate-target distance (cm)	15
Deposition time (min)	90
Rotational speed of specimens (rpm)	5
Substrate bias voltage (V)	-100
Duty cycle (%)	50
Deposition temperature (°C)	200



Figure 1. The classification of coating adhesion according to the VDI3198 standard

2. 3. Corrosion Test The electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) tests using a potentiostat instrument (µAutolab, III/FRA2, made in the Netherlands) were conducted to evaluate the corrosion behavior of uncoated and CrN/CrAlN coated pure Ti and Ti6Al4V alloy substrates in a physiologic Ringer's solution (pH 7.4). The samples were set up according to the conventional three-electrode cell configuration. The EIS tests were operated with a signal amplitude of 10 mV and a frequency ranging from 100000 to 0.01 Hz when the open circuit potential (OCP) was stable, which occurred after 2 hours. The EIS test data were analyzed using NOVA software (version 2.1.3). The PDP test was performed at a scan rate of 1 mV/s, starting from -250 mV below the OCP. The PDP curves were analyzed using the Tafel extrapolation technique. The SEM was applied to study the corrosion surface morphologies characteristics of specimens.

#### **3. RESULTS AND DISCUSSIONS**

**3. 1. Microstructure of the Coating** Figure 2 displays the X-ray diffraction patterns of the Ti substrate and Ti coated with CrN/CrAlN. The latter pattern includes CrN and AlN with a face center cubic (FCC) structure, as well as the Cr2N and substrate with a hexagonal structure. For CrN and AlN phases of this coating, diffraction peaks associated with (111), (200), and (220) planes occur at 37.6, 43.7, and 63.5 angles. On the other hand, diffraction peaks of the titanium are at 35, 38.4, and 40.1 angles in relation to (100), (002), and (101) planes. According to the observed pattern, the coating's referred orientation is (200), consistent with previous researchers' reports (29, 30).

**3. 2. Suface Morphology and Coating Thickness** Figure 3 ehibits the SEM images of the CrN/CrAIN coating urface. Macroparticles can be observed on the



Figure 2. XRD pattern of CrN/CrAlN coating



**Figure 3.** SEM images of CrN/CrAlN surface coating with different magnifications a)  $\times$ 500, b)  $\times$ 1000

surface. The presence of macroparticles is normal in the cathodic arc evaporation process and causes a partial increase in the roughness of the coated samples compared with the uncoated samples. The factors affecting the number and size of microparticles include the rate of evaporation of the target material, the deposition rate, and accumulation of the coating on the metal substrate (31). Figure 4 illustrates the FESEM images of the crosssection of the coating. The images display a continuous and dense coating microstructure. Additionally, the lack of a separation line between the substrate and coating reveals a high adhesion of the coating to the substrate. Moreover, the CrN and CrAlN nanolayers were compactly adhered together, without any visible cracks or holes in their interface resulting in improved corrosion resistance. The created coating possesses a nanostructure with a fully homogeneous, 2-micron thickness, and compact layers of CrN and CrAlN. Figure 5 shows the energy distribution spectroscopy (EDS) of the coated samples. The analysis was performed from the surface to the depth of the sample and includes Cr, Al, N, and Ti elements.

**3. 3. Surface Roughness and Adhesion** The coating adhesion was evaluated via Rockwell-C test in the present investigation. The condition of the coating surrounding the impression of the indenter was observed using an optical microscope. Figure 6 displays the images obtained from the adhesion tests for titanium and Ti6Al4V samples coated with CrN/CrAlN. No cracks or disintegration exist around the impression of the indenter, indicating a high level of coating adhesion in the HF1 group. Table 2 summarizes the surface roughness data for coated and uncoated samples. The coated samples have a higher roughness than the uncoated samples due to the nature of the cathodic arc evaporation process, explained in section 2.3.

**3. 4. Electrochemical Behavior** The corrosion behavior of the titanium and Ti6Al4V substrates before and after being coated with nanolayer CrN/CrAlN



Figure 4. FESEM images of the cross section of CrN/CrAIN coating with different magnifications



**Figure 5.** EDS line analysis of titanium sample with CrN/CrAlN coating



Figure 6. Optical microscope images of the indenter impression on coating  $\times 100$  magnification, (a) commercial pure titanium, and (b) Ti6Al4V

**TABLE 2.** Surface roughness values of uncoated and CrN/CrAlN coated titanium and Ti6Al4V samples

Sample	$R_{a}\left(\mu m\right)$	R <sub>z</sub> (µm)	R <sub>max</sub> (mm)
Titanium	0.169	0.893	0.02
CrN/CrAlN coated titanium	0.221	1.220	0.04
Ti6Al4V	0.125	1.186	0.03
CrN/CrAlN coated Ti6Al4V	0.158	1.374	0.04

coatings was evaluated by EIS and PDP tests in the physiological Ringer's solution. Figure 7 illustrates the EIS test results in the form of Nyquist and Bode plots for uncoated and CrN/CrAlN coated titanium and Ti6Al4V substrates samples.



**Figure 7.** (a) Nyquist and (b) Bode plots of uncoated and CrN/CrAlN coated pure Ti and Ti6Al4V alloy substrates after 2 hours of exposure to physiological Ringer's solution

The Nyquist plots of all uncoated and coated substrates (Figure 7 (a)) showed an uncompleted semicircle-like shape, while those for CrN/CrAlN coatings were larger in diameter. As can be observed in Bode plots of specimens (Figure 7 (b)), the uncoated titanium and Ti6Al4V indicated only one time constant. which is related to the capacitive behavior of the electrical double layer (Cdl) and the charge transfer resistance (Rct) of the surface oxide layer. However, there were two-time constants in Bode plots of the CrN/CrAlN coated samples, representing the capacitive behavior of the coatings and the electrical double layers. Moreover, at high-frequency regions, the frequency independency of the absolute impedance values suggested pure resistance behavior of specimens. The experimental impedance data of the uncoated and CrN/CrAlN coated titanium and Ti6Al4V substrates were fitted utilizing the equivalent circuit models displayed in Figure 8 (a) and (b), respectively. In these models, Rs, Rct, and Rcoat are respectively ascribed to



**Figure 8.** Equivalent circuits used to fit the EIS data of (a) uncoated and (b) CrN/CrAlN coated pure Ti and Ti6Al4V alloy substrates

Ringer's solution resistance, charge transfer resistance (at the interface of substrate/Ringer's solution), and coating resistance (at the interface of coating/Ringer's solution). Moreover, CPEdl and CPEcoat are assigned to the constant phase elements of the electrical double layer and the coating capacitance, respectively. Generally, the CPE is employed in the circuit to compensate for the deviation of Cdl and Ccoat from ideal capacitive behavior due to the surface inhomogeneity (32, 33). The equivalent circuits fitted parameters are reported in Table 3. According to Table 3, it was found that the Rct values of CrN/CrAlN coated titanium and Ti6Al4V substrates (2.27 and 2.09 M $\Omega$ .cm<sup>2</sup>, respectively) were higher than that of the uncoated samples (0.20 and 0.66 M $\Omega$ .cm<sup>2</sup> for titanium and Ti6Al4V substrates, respectively) which indicated improved anticorrosion properties of titanium and Ti6Al4V after being modified with nanolayer CrN/CrAlN coatings. Furthermore, when comparing CrN/CrAlN coated titanium and Ti6Al4V specimens with each other, the former presented higher Rct and lower Rcoat values. The PDP curves of uncoated and CrN/CrAIN coated titanium and Ti6Al4V substrates are indicated in Figure 9. For both titanium and Ti6Al4V substrates specimens, because of the formation of a surface passive oxide layer, the passive behavior was observed. The Ecorr, corrosion current density (icorr), anodic and cathodic slopes (ßa and ßc, respectively), and polarisation resistance (Rp) values of specimens derived from the PDP curves utilizing the Tafel extrapolation technique are summarized in Table 4. The Rp values of specimens were calculated using the Stern-Geary equation (34). While the Ecorr reflects the tendency of

TABLE 3. Simulated EIS parameters for uncoated and CrN/CrAIN coated titanium and Ti6AI4V substartes in physicological Ringer's solution Sample  $R_s(\Omega.cm^2)$  $CPE_{dl}$  (µF/cm<sup>2</sup>)  $R_{ct}$  (MQ.cm<sup>2</sup>)  $CPE_{coat}$  (MQ.cm<sup>2</sup>)  $R_{coat}$  (KQ.cm<sup>2</sup>)  $\mathbf{n}_{dl}$ n<sub>coat</sub> Titanium 100.08 85.42 0.88 0.20 \_ CrN/CrAIN coated titanium 102.98 26.13 0.91 2.27 127.18 0.87 1.30 Ti6AI4V 111.78 38.34 0.93 0.66 -\_ CrN/CrAIN coated Ti6AI4V 102.87 28.44 0.92 2.09 105.02 0.81 2.03

TABLE 4. The Ecorr and icorr values of uncoated and CrN/CrAIN coated titanium and Ti6AI4V substartes					
Sample	$E_{corr}$ (mV)	<i>i<sub>corr</sub></i> (µA/cm <sup>2</sup> )	$\beta_a$	$\beta_c$	$R_p$ (K $\Omega$ .cm <sup>2</sup> )
Titanium	100.08	85.42	0.88	0.20	-
CrN/CrAIN coated titanium	102.98	26.13	0.91	2.27	127.18
Ti6AI4V	111.78	38.34	0.93	0.66	-
CrN/CrAIN coated Ti6AI4V	102.87	28.44	0.92	2.09	105.02



Figure 9. The classification of coating adhesion according to the VDI3198 standard

dissolution and stability, the icorr represents the corrosion rate. So, the lower the icorr and the more positive the Ecorr, the higher the corrosion resistance (29, 31, 35). The Ecorr and icorr values of CrN/CrAlN coated samples were respectively nobler and lower than those of uncoated ones, showing a remarkable enhancement in corrosion resistance of titanium and Ti6Al4V substrates after being coated with nanolayer CrN/CrAlN coatings. Titanium is corroded under the formation of soluble titanium oxychloride complexes and the consumption of the passive oxide layer by Cl– corrosive ions (36). According to Liang et al. (37), the following anodic and cathodic reactions happen during the corrosion of titanium and Ti6Al4V in Ringer's solution: Anodic reactions:

$$Ti + 4Cl^{-} \rightarrow TiCl_{4} + 4e^{-}$$
(1)

 $TiCl_4 + 2H_2O \rightarrow TiO_2 + 4Cl^- + 4H^+$ (2)

Cathodic reaction:

$$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$$
(3)

The CrN/CrAlN coating can act as a barrier against corrosion, not allowing direct contact of the corrosive solution with the titanium substrate. The improved structural density due to the increased number of interfaces in multilayer coatings can significantly enhance the corrosion resistance of the substrate compared with single-layer ones (29, 38). Although the Ti6Al4V substrate possessed a more negative Ecorr value (-405 mV) than that of titanium (-368 mV), the icorr value of Ti6Al4V (0.0278 µA/cm<sup>2</sup>) was lower than the icorr value of titanium (0.0399 µA/cm<sup>2</sup>), suggesting better anticorrosion behavior of Ti6Al4V. The  $\alpha + \beta$  twophase structure of Ti6Al4V with additional Al and V promotes its anodic passivation and increases its corrosion resistance compared with titanium (37). However, after being coated with CrN/CrAlN coatings, titanium exhibited more negative Ecorr (-54 mV) and lower icorr (0.0046  $\mu$ A/cm<sup>2</sup>) values than Ti6Al4V (with Ecorr and icorr values of -28 mV and 0.0086 µA/cm<sup>2</sup>, respectively). Therefore, the corrosion resistance (Rp) of specimens was increased in the following order: uncoated titanium (64.842 KΩ.cm<sup>2</sup>) < uncoated Ti6Al4V  $(93.064 \text{ K}\Omega.\text{cm}^2) < \text{CrN/CrAlN}$  coated Ti6Al4V  $(362.137 \text{ K}\Omega.\text{cm}^2)$  < CrN/CrAlN coated titanium  $(581.472 \text{ K}\Omega.\text{cm}^2).$ 

Figure 10 shows the SEM surface morphologies of CrN/CrAlN coated titanium and Ti6Al4V substrates specimens after the corrosion test. Although some small



**Figure 10.** SEM surface morphologies of CrN/CrAlN coated specimens of (a) pure Ti and (b) Ti6Al4V alloy substrates after the corrosion test

corrosion pits were formed and no crack was seen on both coated surfaces, it seems that the CrN/CrAIN coated titanium underwent less damage compared to the coated Ti6Al4V. This showed the lower corrosion susceptibility of coated titanium in physiological Ringer's solution, as earlier discussed. Pits are formed because the coatings defects including cavities and macroparticles provide a direct path for corrosive ions to contact with the substrate (31-33). It can be concluded that pitting was the main corrosion mechanism of the specimens.

#### 4. CONCLUSION

In this study, arc evaporation method was used to deposit CrN/CrAIN nanolayer coating on titanium and Ti6Al4V substrates. The results from the corrosion behavior evaluation of the coated and uncoated samples in Ringer's solution demonstrated that the deposited coating changed the corrosion potential from -0.386 V to -0.054 V for titanium and from -0.405 V to -0.0287 V for Ti6Al4V. In addition, the current density was reduced to about one-eighth and third for coated titanium and Ti6Al4V samples, respectively. Moreover, the increased capacitator circle diameters due to the deposition of CrN/CrAIN coating indicated improved corrosion behavior of the coated samples compared to the uncoated specimens.

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#### Persian Abstract

در سالهای اخیر از کاشتنیها به عنوان پروتز برای جایگزینی و محافظت از استخوان استفاده می شود. تیتانیوم، به عنوان یک ماده کاشتنی، برای عملکرد بهتر نیاز به بهبود خواص خوردگی و سایش دارد. بنابراین، در مطالعه حاضر پوششهای نیترید با هدف بهبود خواص خوردگی و سایش بر زیرلایه تیتانیومی اعمال شدند. روش رسوب فیزیکی بخار تبخیر قوس کاتدی (CAE-PVD) برای رسوب پوشش های نانولایه CrN/CrAIN بر روی زیرلایههای تیتانیوم خالص تجاری و آلیاژ Ti6Al4V برای کاربردهای بیومواد استفاده شد. از پراش پرتو ایکس (XRD) برای مشخص کردن ساختار بلوری پوشش و از میکروسکوپ الکترونی روبشی (ESEN) و میکروسکوپ الکترونی روبشی نشر میدانی (FESEM) برای مشاهده مورفولوژی سطح و سطح مقطع پوشش استفاده شد. چسبندگی پوشش طبق استاندارد ID48 با استفاده از فرورونده Cokewell-اندازه گیری شد. رفتار خوردگی توسط پلاریزاسیون پتانسیودینامیک و امپدانس الکتروشیمایی طیفسنجی در محلول رینگر ارزیابی شد. نتایج نشان داد که پوشش نانولایه تاندازه گیری شد. رفتار خوردگی توسط پلاریزاسیون پتانسیودینامیک و امپدانس الکتروشیمایی طیفسنجی در محلول رینگر ارزیابی شد. نتایج نشان داد که پوشش نانولایه پتانسیل خوردگی را از V 2080- به V 4000- برای نمونه تیتانیوم و از V 2040- به V 2020- برای نمونه VID444 به جزیان خوردگی برای نمونه های پوشش داده شده تیتانیوم و از از V 2040- به V 2020- برای نمونه VID444 به جزیان خوردگی برای نمونه های پوشش داده شده تیتانیوم و دا ز از V 2040- به V 2020- برای نمونه VID444 با سنفاده از موموراین، چگالی جزیان خوردگی برای نمونه های پوشش داده شده تیتانیوم و دا ز از V 2040- به V 2020- برای نمونه VID444 رومبراین، چگالی جزیان دخوردگی برای نمونه های پوشش داده شده تیتانیوم و در آن به حدود یک هشتم و یک سوم کاهش یافت. قطر دایره خاز به دلیل رسوب پوشش مانعی در برابر نفوذ دروردگی معلی می نشان دهنده رفتار خوردگی بهبود یافته نمونههای پوشش داده شده در مقایسه با نمونه های بدون پوشش است، زیرا پوشش به عنوان مانعی در برابر نفوذ محلول خورنده به زیرلایه عمل می کند.

*چکیدہ* 



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# Optimization of Operating Parameters of a Scroll Expander Based on Response Surface and NSGA II

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#### ABSTRACT

Adjusting the operating parameters to optimize the performance of the scroll expander has been a hot research topic among scholars. This paper innovatively combines the response surface method and NSGA2 algorithm for parameter optimization. This novel method can accurately predict the optimal operating parameters of the scroll expander and improve the overall efficiency of the scroll expander. Initially, a three-dimensional transient simulation model of the scroll expander was established, and the effects of three key operating parameters (suction pressure, exhaust pressure, and rotational speed) on the output power and isentropic efficiency of the scroll expander were analyzed through numerical simulation. On this basis, the response surface model between the input parameters and the objective function was established by using the response surface methodology. Consequently, three different optimization algorithms were compared, and it was found that NSGA-II had a better performance both in terms of convergence and solution performance,. Threfore, the NSGA-II algorithm was used for the multi-objective optimization. Under the premise of considering the maximum output power and isentropic efficiency, based on the established response surface model, the Pareto optimal solution was used to determine the optimal combination of its operating parameters: suction pressure of 1.62 MPa, exhaust pressure of 0.45 MPa, and rotational speed of 2,099.58 rpm.Finally, the numerical model is verified by the laboratory-built test bed of the Organic Rankine cycle low-temperature waste heat oilfree power generation system. The experimental results match well with the numerical simulation results and verify the model accuracy. The results from this pioneering and thorough thr study will provide a solid benchmark for the development and refinement of upcoming scroll machines.

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#### **1. INTRODUCTION**

With the intensive research on scroll expanders, many scholars have attempted to improve the performance of scroll expanders by changing the geometry. Fanti et al. (1) investigated tooth side gap size on the features of vortex expanders. Alshammari et al. (2) used new mathematical models to improve the scroll expander's profile. Gao et al. (3) developed a new expander. It was shown that this design has better performance than conventional expanders.

As Computational Fluid Dynamics technology continues to evolve, the investigation into the internal flow field within the expander is garnering increasing interest among academic researchers. Feng et al. (4) used the custom way to solve the vortex motion problem. Emhardt et al. (5) constructed a Vortex Swellers with variable wall thickness. Emhardt et al. (6) used new way to analyze the effect of variable Vortex Swellers. Zheng et al. (7) investigated the effect of the resolution of the CO<sub>2</sub> property table on the numerical simulation. Song et al. (8) proposed a symmetric exhaust structure of Vortex Swellers. Singh et al. (9) proposed symmetric exhaust structure of a Vortex Swellers. Song et al. (10) performed three-dimensional numerical simulations of a Vortex Swellers with different suction port positions based on CFD. Du et al. (11) compared the performance differences between T-CO<sub>2</sub> and R123. CO<sub>2</sub> and R123 performance differences, T-CO<sub>2</sub> exhibited better performance with an average isentropic efficiency 14% higher than that of R123.

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With improvement of experimental conditions, more and more scholars also focus on the experimental study of vortex expanders. Zhang et al. (12) conducted an experimental study of vortex expanders at 65C-96°C and compared the effects of the work mass, Fatigati et al. (13) compared the difference in the performance of vortex expander and slide rotary expander on ORC respectively. Hsieh et al. (14) developed a new ORC using R123a as the work material and experimentally investigated the performance of expander. Oh et al. (15) developed a new model of a Vortex Swellers, and through the coupling of the simulation model with the experimental vales, two key unknown parameters were identified. Jalili et al. (16) conducted research on the effect of carbon nanotube (CNT) particles on refrigeration cycle performance. They conducted specific and rigorous experiments. Vanaei et al. (17) conducted an evaluation and refinement of an altered incineration facility through the Organic Rankine Cycle.

Upon a thorough analysis of the research synopsis presented above, it can be inferred that output power and isentropic efficiency serve as pivotal metrics for assessing the operational efficacy of a scroll expander. These two key variables do not operate in a vacuum; instead, they are shaped by various factors, such as pressure, speed, and the distinct geometry of the scroll expander. Nevertheless, existing studies typically concentrate on examining the impact of a solitary factor on the performance of Vortex Swellers, leaving a noticeable gap in the comprehensive discussion on the adjustment of these operating parameters for performance optimization. Consequently, this study employs numerical simulation to conduct an allencompassing investigation of the three operating parameters of Vortex Swellers, aiming to identify optimal parameters for real-world operation. Most notably, we introduce a novel optimization method, which combines the response surface methodology and the NSGA II algorithm to facilitate in-depth multiobjective optimization. This approach allows us to derive optimal operating parameters for the Vortex Swellers. The findings from this innovative and comprehensive study will offer a robust reference point for the design and enhancement of future scroll machines.

#### 2. MODELING

**2. 1. Geometric Modeling of a Vortex Expander** The design of the Vortex Swellers's profile is informed by circular involutes, with the tooth head correction relying on double arc correction. Figure 1 provides a visual representation of the Vortex Swellers's geometric model, while Table 1 lays out the specific geometric parameters in detail.



Figure 1. Geometric model of vortex expander

TABLE 1. Scroll expander geometric parameters					
Definition	Parameters	Units	Value		
Base circle radius	R	mm	4.647		
Center distance	r	mm	9.6		
Height of tooth	h	mm	42.5		
Wall thickness	t	mm	5		
Involute angle	а	0	30.767		

**2. 2. Turbulence Model** The continuity equation can be obtained by the following formulas (18).

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} - S_{add} = 0$$
(1)

where P denotes mass per unit volume, t signifies temporal duration and  $u_x v_x w$  are speeds corresponding to the  $x_x y_x z$  axis, respectively.  $S_{add}$  embodies the accumulated mass in the continuous and any customdefined origins. with a default value of 0.

The energy conservation equation can be obtained by the following formulas (19).

$$\frac{\partial}{\partial t} \left( \rho \left( U + \frac{v^2}{2} \right) \right) + \nabla \cdot \left( \rho v \left( h + \frac{v^2}{2} \right) \right) =$$

$$\nabla \cdot \left( \lambda_{eff} \nabla T - \sum_j h_j \vec{J}_j + \tau_{eff} \cdot \vec{v} \right) + S_{\text{volume}}$$
(2)

$$U = h - \frac{p_{op} + p}{\rho}, h = c_p dT + \frac{p}{\rho}$$
(3)

where  $\lambda_{\text{eff}}$  signifies the efficient transfer capacity,  $\overline{J}_{j}$  alludes to the dispersion flow of the compound, U characterizes the intrinsic energy within the compound, h marks the perceptible heat content,  $\tau_{eff}$  highlights the tension matrix,  $p_{op}$  pertains to the functional atmospheric force, P is the relative atmospheric force, and  $S_{\text{volume}}$  designates the bulk warmth origin.

**2. 3. Vortex Expander Output Characteristics** Equation for the output power of Vortex wellers (20):

$$\overline{M} = \int_{t}^{t+T} M_{t}(t) dt = \int_{t}^{t+T} F_{t} \cdot \mathbf{r} dt$$
(4)

$$W = \frac{2\pi n}{60}\overline{M} \tag{5}$$

where *n* signifies the spin frequency,  $\overline{M}$  stands for the averaged momentum over time of the circulating scroll,  $F_t$  is the tangential force on the moving scroll disk, and *r* alludes to the foundational circle's diameter.

Equation for the isentropic efficiency of a vortex expander can be obtained by the following formulas (21):

$$\eta = \frac{H_1 - H_2}{H_1 - H_2} = \frac{W}{\overline{m}(h_{\rm in} - h_{\rm out})}$$
(6)

where  $\overline{m}$  represents the weight flux of the operational liquids over a time interval,  $h_{in}$  designates the articular heat content at the entry point of these liquids, and  $h_{out}$  points to the particular heat content at the exit point of these operational liquids.

**2. 3. Meshing** The role of meshing is particularly important in computational fluid dynamics (CFD) analysis, which largely determines the accuracy and convergence of subsequent numerical simulations. ANSYS Fluent software will be used to perform numerical simulations. Taking the vortex expander as an example, a specific meshing strategy can effectively characterize the fluid region model of the vortex expander. Typically, a hybrid meshing strategy is used to model the fluid region of a vortex expander. This hybrid meshing approach is designed to maximize the reflection of the fluid flow characteristics inside the vortex expander. Figure 2 illustrates the mesh model.

**2. 4. Grid Sensitivity Validation** In order to select the appropriate grid scale and number of computational domain grids, the numerical calculation results of five different numbers of grid models for



Figure 2. Meshing model

specific operating conditions were compared and the results are shown in Table 2. When comparing A3 grid to A1 grid and A2 grid, we found that their deviations in mass flow rate, driving moment and isentropic efficiency are less than 6%. While comparing the A3 grid to the A4 grid and A5 grid, we can observe that the deviations in mass flow rate, driving moment and isentropic efficiency are less than 8%. Considering the accuracy and efficiency together, A3 grid has met the requirements of grid independence and computational accuracy when performing the numerical simulation of the vortex expander.

#### **3. ANALYSIS OF RESULTS**

**3. 1. Effect of Different Exhaust Pressures on the Performance of Scroll Eexpanders** We selected four distinct exhaust pressures for examination, with Table 3 detailing the specific working conditions associated with each other.

Figure 3 portrays the changes in isentropic efficiency and exported energy of the scroll expander under varying exhaust pressures. A close examination of Figure 3 reveals that an increase in exhaust pressure results in divergent trends for output power and isentropic efficiency. Specifically, exported energy decreases while isentropic efficiency increases. This is linked to the fact that the scroll expander's exported energy is influenced by the pressure differential between the inlet and outlet. An increase in exhaust pressure reduces this differential.

**TABLE 2.** Time-averaged performance of vortex expanders with different number of grids

Grid level	Total number of grids	Mass flow (kg/s)	Torques (N.m)	Isentropic efficiency (%)	Times (s)
A1	55E+4	0.11658	5.12	36.52	8h
A2	85E+4	0.12458	5.42	37.82	16h
A3	110E+4	0.12796	5.64	38.16	23h
A4	150E+4	0.13124	5.83	38.64	33h
A5	210E+4	0.13216	5.89	38.94	44h

**TABLE 3.** Different exhaust pressure parameters

Condition number	Suction pressure (MPa)	Inlet temperature (K)	Exhaust pressure (MPa)	Rotation speed (r/min)
S1	1.2	400	0.15	2000
S2	1.2	400	0.3	2000
<b>S</b> 3	1.2	400	0.45	2000
S4	1.2	400	0.6	2000

Consequently, with a smaller pressure difference, the gas's capability to transform energy into mechanical work during expansion is restricted, leading to a reduction in the vortex expander's output power. On the other hand, a higher exhaust pressure decreases the pressure drop, which facilitates a more efficient conversion of pressure energy into kinetic energy. In addition, a moderate exhaust pressure helps to maintain a more stable flow velocity distribution and reduces the energy loss due to turbulence. In the actual expansion process, irreversible losses occur due to friction, turbulence, and non-uniform distribution of fluid pressure, leading to an increase in entropy (22). When the exhaust pressure is moderately increased, these irreversible losses are reduced; thus, increasing the isentropic efficiency.

The transient variation of the exported energy of the scroll expander at different exhaust pressures is given in Figure 4. Exported energy transient curve shows a downward flat trend Upon increasing the exhaust pressure as it goes from 0.15 MPa to 0.60 MPa. The exhaust pressure significantly affects the degree of gas expansion within the vortex expander, which in turn affects the output power. At lower exhaust pressures, the gas has to undergo a greater degree of expansion, releasing more energy and leading to an increase in output power. Conversely, at higher exhaust pressures, the gas expands less, releasing less energy and reducing the power output. Therefore, the magnitude of fluctuations in the output power transient plots and the average exported energy may vary under different exhaust pressure conditions.

# **3. 2. Effect of Different Suction Pressures on the Performance of Vortex Expanders** We maintained a constant inlet temperature for the Vortex Swellers's working mass, while varying the suction pressure. Table 4 presents the parameters pertaining to these simulated working conditions.



Figure 3. Isentropic efficiency and output power diagram for different exhaust pressure



Figure 4. Variation of output power under different exhaust pressure

TABLE 4. Different suction pressure parameters

Condition number	Suction pressure (MPa)	Inlet temperature (K)	Exhaust pressure (MPa)	Rotation speed (r/min)
T1	0.8	400	0.25	2000
T2	1.1	400	0.25	2000
T3	1.4	400	0.25	2000
T4	1.7	400	0.25	2000

As latter escalates from 0.8 MPa to 1.7 MPa, the former sees a clear upward trend, moving from 1.074 kW to 3.056 kW. The underlying reason for this trend is the increased gas density with the rise in suction pressure. This enables Vortex Swellers to extract more energy from the gas, leading to an increment in output power. Figure 5 shows the isentropic efficiency and output power for different suction pressure. When assessing the isentropic efficiency in relation to suction pressure, a subtle increase is noticed as the suction pressure moves from 0.8MPa to1.1MPa. In contrast,



Figure 5. Isentropic efficiency and output power for different suction pressure
between 1.1MPa and 1.7MPa, the isentropic efficiency reveals a decline, falling from 37.6% to 32.1% - a total reduction of 5.5%.

Figure 6 illustrates the temporal changes in the Vortex Swellers 's output power at various suction pressures. It is evident from the figure that the output power increases in line with the rise in suction pressure. This allows more fluid to participate in the expansion process per time unit, leading to a greater conversion of pressure energy into rotational energy in the moving scroll disk, and thereby enhancing the scroll expander's output power.

# **3. 3. Effect of Different Rotational Speeds on the Behavior of Vortex Expanders** Specific parameters are shown in Table 5.

An inspection of Figure 7 reveals that within the speed range of 1200rpm-2100rpm. The output power escalates from 1.27kW to 2.07Kw, marking a growth rate of 62.9%, whereas the isentropic efficiency moves up from 25.5% to 37.7%, indicating a growth rate of 47.8%.

Figure 8 provides the transient diagrams of the scroll expander's energy output at varying speeds. A perusal of Figure 8 reveals that at lower speeds, the export of energy experiences less fluctuation in the range of  $1.9\pi$  to  $2.2\pi$ , maintaining an overall steady trajectory. However, at higher speeds, the output power exhibits t



Figure 6. Transient curve of output power at different suction pressure

TABLE 5. Different exhaust pressure parameters

Condition number	Suction pressure (MPa)	Inlet temperature (K)	Exhaust pressure (MPa)	Rotation speed (r/min)
1	1.2	400	0.25	1200
2	1.2	400	0.25	1500
3	1.2	400	0.25	1800
4	1.2	400	0.25	2100



Figure 7. Graph of Isentropic efficiency and export of energy for different speeds



Figure 8. Transient diagram of output power at different speeds

more significan fluctuations, with a discernible downward trend. This can be attributed to the following reasons: In the scroll expander's low rotational speed phase, the gas expands slowly, resulting in a larger decrease in internal energy. This causes the export of energy to incrementally increase with the rise in rotational speed. As the Vortex Swellers moves into the mid-speed phase, the gas expansion speed picks up, the internal energy decreases, and the export of energy transient curve displays a slow growth, gradually stabilizing. However, in the high-speed phase, the gas expands too quickly, and the reduction in internal energy is limited. This results in the output power reaching a peak as the speed increases, after which an evident decline is observed.

# 4. MULTI-OBJECTIVE OPTIMIZATION

**4. 1. Response Surface** Its main function is to form a response function that characterizes in detail the

interrelationships between input and output variables. This objective function can usually be expressed as an equation of the following form:

$$Y_{i} = \beta + \sum_{i=1}^{k} \beta_{i} x_{i} + \sum_{i=1}^{k} \beta_{ii} x_{ii}^{2} + \sum_{i=1}^{k} \sum_{j>1}^{k} \beta_{ij} x_{i} x_{j}$$
(7)

We chose to adopt BBD for the experimental design of this study. Table 6 lists the parameters of BBD design.

**4. 1. ANOVA and Regression Models** The magnitude of F-value is opposite to the magnitude of P-value. As shown in the Table 8, F of the model is 237.5 and P is less than 0.0001, these values indicate that the significance of our constructed model is very strong. In assessing the accuracy of the model,  $R^2$  and  $R_{adj}$  important reference indicators. The closer the values of these two metrics are to 1 and the smaller the gap between them is, it means that the model is more

TABLE 6. Three-factor design table

Code	Variables	Level				
	variables	-1	-1 0 1			
А	Suction pressure	0.8	1.3	1.8		
В	Exhaust pressure	0.15	0.375	0.6		
С	Rotation speed	1200	1600	2100		

accurate. In the table,  $R^2$  is 0.9967 and  $R_{adj}$  is 0.9925, which are both very close to 1, and the difference between them is only 0.0042, these values fully indicate that our model has a very high accuracy. From Table 9 we can find that  $R^2$  is 0.9913 and Radj is 0.9807, both which are close to 1, highlighting the model's ability to accurately reflect changes in isentropic efficiency. At the same time, the small difference of only 0.0106 strongly confirms the high accuracy of the model.

The fitted curves are expressed as Equations 8 and 9. W = -0.5636 + 1.1353A - 0.3088B - 0.001C + 0.8449AB + $0.0009AC - 0.004BC - 0.3835A^2 - 2.9686B^2 + 1.0833e-8C^2$ (8)

$$\eta = -0.2366 - 0.3676A - 0.3938B + 0.0002C + 0.2769AB - 0.0024AC + 0.0006BC - 0.1135A^2 - 0.9037B^2 - -5.7451e - 8C^2$$
(9)

**4. 2. Response Surface Result Analysis** In the response surface plot shown in Figure 9, we can find that the output power is at a low level at the combination of horizontal intervals of suction pressure taking the value range of 0.8-1.2 MPa and exhaust pressure taking the value range of 0.5-0.6 MPa. However, the output power is at a high level at the combination of horizontal intervals for the range of values of suction pressure 1.6-1.8 MPa and the range of values of exhaust pressure 0.15-0.3 MPa.

<b>TABLE 7.</b> Three-factor, three-level parameter design table	e
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3	Suction pressure (MPa)	Exhaust pressure (MPa)	Rotation speed (r/min)	Output power	Isentropic efficiency
	Α	В	С	( <b>kW</b> )	(%)
S1	0.8	0.4	2000	0.683	40.5
S2	1.3	0.375	2000	2.312	33.4
<b>S</b> 3	1.3	0.4	1600	1.599	37.9
S4	1.8	0.15	1600	2.736	26.1
S5	1.8	0.4	1300	2.033	30.3
S6	1.8	0.6	1600	1.999	38.6
<b>S</b> 7	1.8	0.4	2000	2.982	40.6
S8	0.8	0.375	2000	1.074	36.2
S9	1.1	0.15	2000	1.843	37.6
S10	1.4	0.25	2000	2.504	35.6
S11	1.8	0.25	2000	3.053	32.1
S12	1.2	0.15	1600	2.123	28.4
S13	1.3	0.375	2000	1.811	36.4
S14	1.2	0.45	2000	1.591	45.5
S15	1.2	0.6	1200	1.095	49.4
S16	1.3	0.25	1200	1.276	25.5
S17	1.2	0.15	1600	1.598	30.8

Source	Sum of Squares	df	Mean Square	<b>F-value</b>	p-value
Model	7.27	9	0.8074	237.35	< 0.0001
А	0.6234	1	0.6234	183.26	< 0.0001
В	0.1297	1	0.1297	38.14	0.0005
С	0.1054	1	0.1054	30.99	0.0008
AB	0.0052	1	0.0052	1.52	0.2576
AC	0.0255	1	0.0255	7.49	0.0291
BC	0.0004	1	0.0004	0.1238	0.7353
A <sup>2</sup>	0.0152	1	0.0152	4.48	0.0720
B <sup>2</sup>	0.0331	1	0.0331	9.72	0.0169
C <sup>2</sup>	4.622E-06	1	4.622E-06	0.0014	0.9716
Residual	0.0238	7	0.0024		
Lack of Fit	0.114	10	0.0034		
Pure Error	0.001	1	0.0023	4.541	0.362
Cor Total	7.29	16	0.0018		
R <sup>2</sup> =0.9967		R <sub>adj</sub> =0.9925		C.V%=3.07	

**TABLE 8.** Output power analysis of variance table

**TABLE 9.** Isentropic efficiencyanalysis of variance table

Source	Sum of Squares	df	Mean Square	<b>F-value</b>	p-value
Model	1474.36	9	147.43	91.43	< 0.0001
A-pin	16.28	1	16.28	1.11	0.3274
B-pout	216.86	1	216.86	13.19	0.0084
C-N	68.46	1	68.46	58.88	0.0001
AB	32.16	1	32.15	6.81	0.0349
AC	8.64	1	8.64	3.56	0.1013
BC	3.86	1	3.86	9.88	0.0163
A <sup>2</sup>	2.68	1	2.68	16.41	0.0049
B <sup>2</sup>	4.42	1	4.42	37.64	0.0005
C <sup>2</sup>	6.46	1	6.46	1.60	0.2468
Residual	122.24	7	7.86		
Lack of Fit	120.68	11	9.48		
Pure error	0.12	1	0.18		
Cor Total	1842.68	16			
R <sup>2</sup> =0.9916		$R_{adj}$ =0.9807		C.V%2.55	

As shown in Figure 10, it can be found that the fluctuation of the surface in the direction of suction pressure is large, while the fluctuation of the surface in the direction of speed is relatively small. This indicates that the effect of suction pressure on the output power is more significant compared to the effect of rotational speed. This finding is important for practical applications because the researcher can maximize the output power by adjusting the combination of suction pressure and rotational speed. The output power falls in

the optimum range when the suction pressure is 1.6MPa-1.8MPa and the rotational speed lies in the range of 1850-2000rpm.

Figure 11 demonstrates the response surface plots of the output power as a function of exhaust pressure and rotational speed. Observing Figure 11, we can find that when the exhaust pressure is in the range of 0.15MPa-0.33MPa, the trend of output power reduction is more obvious as the exhaust pressure decreases. However,



Figure 9. Response surface of output power under the interaction of suction pressure and exhaust pressure



Figure 10. Response surface of output power under the interaction of suction pressure and rotational speed

when the exhaust pressure is at 0.33MPa-0.60MPa, the trend of output power reduction is relatively slower as the exhaust pressure decreases. This indicates that at different exhaust pressure intervals, the output power has different sensitivities to changes in exhaust pressure.



Figure 11. Response surface of output power under the interaction of exhaust pressure and rotational speed

The interaction between response surface and contour visuals, as depicted in Figure 12, demonstrates the trend of isentropic efficiency under varied inlet and exhaust pressure conditions. This analysis suggests that notable enhancement in isentropic efficiency can be achieved when the intake pressure is set between 1.6-1.8 MPa and the exhaust pressure falls within the 0.5-0.6 MPa range. This finding bears significant implications, serving as a valuable guide for optimizing the configuration of suction and exhaust pressures to boost the isentropic efficiency of the machinery in real-world applications.

The response surface as shown in Figure 13 reveals in detail the variation characteristics of isentropic efficiency under different conditions of intake pressure and rotational speed. Based on the data analysis in Figure 13, we can conclude that the optimal performance interval of isentropic efficiency is concentrated in the range of 1.1-1.3 MPa intake pressure and 1800-2000 rpm rotational speed under the consideration of only two influencing factors, namely, intake pressure and rotational speed.

The response surface shown in Figure 14 reflects the changing law of isentropic efficiency under different



Figure 12. Isentropic efficiency response surface under the interaction of suction pressure and exhaust pressure



Figure 13. Isentropic efficiency response surface for the interaction of suction pressure and rotational speed



Figure 14. Isentropic efficiency response surface under the interaction of exhaust pressure and rotational speed

exhaust pressure and rotational speed conditions. We can conclude that the isentropic efficiency can reach the optimal parameter range when the exhaust pressure is about 0.51-0.6 MPa and the rotational speed is in the range of 1600-2000 rpm.

4. 3. Performance Comparison of Algorithms To identify the best operational parameters, this research contrasts three frequently employed multiobjective optimization algorithms (MOPSO, NSGA-II, MOEA/D). Eventually, we settle on the NSGA-II algorithm as the most compatible with our model. Figure 15 provides the Pareto optimal solution set diagrams for the three optimization algorithms. The allocation of decision variables for these three optimization algorithms is depicted in Figure 16. From Figure 15, the NSGA-II algorithm has a more concentrated non-inferior solution set and a better diversity of solutions, and the solution set covers all regions of the solution space, which means that we can choose between solutions to satisfy different priorities and preferences. Algorithms with centralized and dense non-inferior solution sets tend to have better convergence. This means that the algorithms are able to find better solutions in a shorter time, which improves the efficiency of solving the optimization problem.

From Figure 16, the MOPSO algorithm as a whole has a more decentralized distribution of decision variables, which presents an unconcentrated character. This means that in the solution space, the MOPSO algorithm is not able to search better for excellent solutions in multiple regions, and the convergence and diversity performance is average (23). The NSGA-II has a fairly uniform distribution of decision variables on the whole, and exhibits better convergence. This indicates that the algorithm is able to effectively find a set of excellent solutions in the solution space with a strong search capability. Compared to the other two algorithms (NSGA II and MOPSO), the MOEA/D algorithm has a wider distribution of decision variables on exhaust pressure, which is mainly concentrated in the range of 0.1MPa-0.55MPa. This implies that the algorithm has a more comprehensive search capability in the exhaust pressure direction and is able to find more potentially excellent solutions. However, in the direction of suction pressure, the distribution of decision variables of the MOEA/D algorithm does not perform well.

In order to better and comprehensively evaluate the advantages and disadvantages of the three algorithms, we introduced HV, IGD, and computation time at the same time for comprehensive evaluation, and the values of the specific evaluation indexes are given in Table 10. Larger HV values and smaller IGD values indicate better performance of the algorithms, and we can see from the table that NSGA-II has obvious advantages over the other two algorithms in terms of HV, IGD, and computation time.

Equation 10 gives the range of values of the independent variables, and for subsequent optimization, the result of the NSGA-II algorithm are given Table 11.

 $\begin{array}{l} Maximize : \text{output power} = f_1(P_{\text{in}}, P_{\text{out}}, n); \\ Maximize : \text{Isentropic efficiency} = f_2(P_{\text{in}}, P_{\text{out}}, n). \\ 0.8MPa \leq P_{\text{in}} \leq 1.8MPa; \\ 0.15MPa \leq P_{\text{out}} \leq 0.6MPa; \\ 1200rpm \leq n \leq 2100rpm. \end{array}$  (10)





Figure 16. Distribution of decision variables for three multi-objective optimization algorithms

**TABLE 10.** Table of performance indicators of the three algorithms

Algorithms	HV	IGD	calculation time (s)
MOPSO	0.9168	1.7569	12.96
NSGA-II	0.9412	1.6686	8.59
MOEA/D	0.9356	2.4214	51.86

<b>IABLE II.</b> Main parameters of NSGA-II algorithm	TA	<b>BLE 11.</b> Main	parameters of NSGA-II algorithm
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Parameters	Values	
Population size	150	
Crossover probability	0.9	
Mutation probability	0.02	
Maximum generation size	500	

By running the NSGA-II algorithm, we obtained a set of Pareto solutions as shown in Figure 17. This set of solutions demonstrates the trade-offs between different objective functions, thus providing diversified choices for decision makers. Point C in Figure 17 is the desired ideal point, where the output power is 3.02 kW, the efficiency is 42.6%, and the optimal operating parameters are: suction pressure is 1.62 MPa, exhaust pressure is 0.45 MPa, and the rotational speed is 2099.58 rpm. The optimal operating parameters solved by the NSGA II algorithm are compared with the simulated values to determine the accuracy of the solution, and the results in Table 12. gives the comparison results. From Table 12, the predicted value of the output power solved by the NSGA II algorithm is

3.02 kW, and the simulated value calculated by numerical simulation is 3.16 kW, with a deviation of 4.4%, and the predicted value of the isentropic efficiency is 42.6%, and the simulated value is 45.4%, with a deviation of 6.2%. The deviation of both is less than 8%, which shows the high accuracy of the optimal solution

# **5. EXPERIMENTAL VALIDATION**

To validate the reliability of the vortex expander's numerical simulation outcomes, we juxtaposed the predicted data with the findings from our experimental setup. Figure 18 provides an intricate depiction of the testing platform. At the heart of this setup is the scroll expander, adapted from an oil-free scroll compressor.



Figure 17. Pareto front plot of NSGA II algorithm

TABLE 12. Comparison of predicted values and simulations

Suction pressure	Exhaust pressure	khaust pressure Rotation		wer (kw)	Isentropic ef	ficiency (%)
(mpa)	(mpa)	speed (rpm)	Predicted value	Simulated value	Predicted value	Simulated value
1.62	0.45	2099.58	3.02	3.16	42.6	45.4

Complementing this, the apparatus incorporates a specialized mass flow pump. It's further outfitted with an evaporator and condenser, each tasked with the vaporization and liquefaction of the working mass, respectively. For precise oversight, we have integrated a smart electromagnetic flow meter. This instrument continuously captures the mass flow rate, enabling meticulous oversight and precision throughout the experimentation phase.

To calibrate the measuring equipment, the following preparations are made:

(1) Make sure that the components of the ORC system are installed and well connected. Make sure the voltmeter is connected correctly and securely to avoid errors or accidents. Connect the ammeter in series with the generator output circuit. Typically, this means that the circuit needs to be disconnected and the two probes of the ammeter connected at each end of the disconnect. Make sure the ammeter is properly and securely installed during installation.

(2) System initialization and preheating: Start the work pump to circulate the work through the system. Start the heater and gradually increase the temperature of the evaporator to evaporate the work mass. During

this process, pay attention to monitor the readings of each measuring instrument to ensure that the working parameters are within the safe range.

(3) Adjustment of suction pressure: Before starting the experiment, select the appropriate suction pressure according to the expected test range. The inlet pressure can be changed by adjusting the frequency of the work pump

(4) After adjusting the suction pressure, wait for the system to reach a stabilized condition. During this time, continuously monitor the readings of each measuring instrument to ensure that the operating parameters remain within the expected range. At the same time, record the suction pressure, temperature, and other parameters of scroll expander at this time.

Figure 19 depicts the schematic diagram of the experiment. The test implementation process strictly adheres to the provisions in the Organic Rankine Cycle Power Generation Unit (JB/T13305-2017)

All experimental data are averaged over several measurements to ensure the reliability of the data.

Firstly, we adjust the inlet pressure into the vortex expander by changing the operating frequency of the work pump.



Figure 18. Experimental platform diagram



Figure 19. Experimental schematic

Secondary, we monitor in real time the voltage and current flowing through the scroll expander. Based on these parameters, we can calculate the export of energy of the scroll expander.

Finally, we compare experimental output power values at different inlet pressures with the simulated values.

Figure 20 shows the experimental values of voltage and current flowing through the scroll expander at different inlet pressures, as measured by our experimental platform. These data are an important basis for analyzing and understanding the operating conditions of the scroll expander.

Figure 21 shows the experimental and simulated output power values. The maximum deviation in output power is 10.86% at a suction pressure of 1.1 MPa. Overall, the deviation between the simulated and experimental results is between 3% and 11%, which constitutes a relatively small deviation. This indicates that model we established is relatively accurate and can effectively simulate the operating characteristics of the scroll expander under different operating conditions.

Meanwhile, we also measured the experimental and simulated values of isentropic efficiency. Figure 22 shows the experimental and simulated values of isentropic efficiency at different suction pressures. The maximum error occurs when the inspiratory pressure is 0.8 MPa, and the maximum error is 12.7%. The reasons for this deviation may be the existence of certain errors in the actual measurement process, the friction loss of the machine and other factors.



Figure 20. Experimental current-voltage diagram at different suction pressures



Figure 21. Simulated versus experimental values of output power



Figure 22. Experimental and simulated values of isentropic efficiency at different suction pressures

# 6. CONCLUSION

Distinct from the research undertakings of prior scholars regarding the operational parameters of the scroll expander, the majority have primarily focused on discerning the extent to which these parameters impact the generated energy and adiabatic effectiveness of the device. Significantly, some academics have deliberated on the optimal configuration of these parameters to ensure peak performance of the scroll expander. This study introduces a methodological fusion of the response surface technique and the NSGA-II algorithm, achieving the optimal operational parameters for the scroll expander. Under these parameters, the scroll expander's performance is comprehensively maximized. The accuracy of this innovative approach has been rigorously validated using a specially constructed experimental platform. Renowned for its high precision and rapid problem-solving capabilities, this novel methodology presents a fresh theoretical framework and perspective for the optimization of the scroll expander. The specific conclusions are as follows:

(1) As the exhaust pressure increases, the pressure difference at the inlet side of the scroll expander decreases, resulting in a lower mass flow rate at the inlet side. Due to the internal structure of the scroll expander, the mass flow rate at the outlet side remains essentially the same as the mass flow rate at the inlet side. A rise in exhaust pressure from 0.15 MPa to 0.60 MPa leads to contrasting trends in the generated energy and adiabatic effectiveness: there's a reduction in output power by 47.17%, while the isentropic efficiency surges by 73.94%. The output power shows a linear increase with the increase of suction pressure. An increase in suction pressure from 0.8 MPa to 1.7 MPa results in a rise in output power by 1.982 kW.the isentropic efficiency shows an initial increase and then a decrease due to factors such as friction and turbulence. When the speed is in the range of 1200 rpm to 2100 rpm, both the

isentropic efficiency and the output power increase with the increase in speed.

(2) The NSGA-II algorithm is more suitable for the multi-objective optimization model both in terms of convergence and solution performance. The maximum export power and isotropy efficiency of the Vortex Expander are derived from solution to be 3.02 kW and 42.6%, respectively, with deviations of 4.4% and 6.2% from the simulated values. The optimum operating parameters: suction pressure, exhaust pressure and rotational speed were 1.62MPa, 0.45MPa and 2099.58rpm.

(3) The accuracy of our method is verified by the organic Rankine cool thermal waste energy production system built in laboratory. The maximum deviations of the experimental values of export power and isotropy efficiency from simulated values are 10.86% and 12.7%, respectively, and the errors are lower than 13%, indicating that the method has relatively better accuracy and can be applied to the actual manufacture. The reasons for this deviation may be the existence of certain errors in the actual measurement process, the friction loss of the machine and other factors.

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#### Persian Abstract

چکیدہ

تنظیم پارامترهای عملیاتی برای بهینهسازی عملکرد گسترشدهنده اسکرول یک موضوع تحقیقاتی داغ در بین محققان بوده است. این مقاله به طور خلاقانه ای روش سطح پاسخ و الگوریتم NSGA2 را برای بهینه سازی پارامتر ترکیب می کند. این روش جدید می تواند پارامترهای عملیاتی بهینه گسترش دهنده اسکرول را با دقت پیش بینی کند و کارایی کلی گسترش دهنده اسکرول را بهبود بخشد. در ابتدا، یک مدل شبیه سازی گذرا سه بعدی از گسترش دهنده اسکرول ایجاد شد و اثرات سه پارامتر عملیاتی کلیدی (فشار مکش، فشار اگزوز و سرعت چرخش) بر توان خروجی و راندمان همسانتروپیک گسترش دهنده اسکرول از طریق عددی مورد تجزیه و تحلیل قرار گرفت. شبیه سازی. بر این اساس، مدل سطح پاسخ بین پارامترهای ورودی و تابع هدف با استفاده از روش سطح پاسخ ایجاد شد. در نتیجه، سه الگوریتم بهینهسازی مختلف با هم مقایسه شدند و مشخص شد که مدل سطح پاسخ بین پارامترهای ورودی و تابع هدف با استفاده از روش سطح پاسخ ایجاد شد. در نتیجه، سه الگوریتم بهینهسازی مختلف با هم مقایسه شدند و مشخص شد که مدل سطح پاسخ بین پارامترهای ورودی و تابع هدف با استفاده از روش سطح پاسخ ایجاد شد. در نتیجه، سه الگوریتم بهینهسازی مختلف با هم مقایسه شدند و مشخص شد که مدل سطح پاسخ جین پارامترهای ورودی و تابع هدف با استفاده از روش سطح پاسخ ایجاد شد. در نتیجه، سه الگوریتم بهینهسازی مختلف با هم مقایسه شدند و مشخص شد که مدل سطح پاسخ جین پارامترهای ورودی و تابع هدف با استفاده از راه حل بهینه پارتو برای تعیین ترکیب بهینه پارامترهای عملیاتی آن استفاده شد. نظر گرفتن حداکثر توان خروجی و راندمان ایزنتروپیک، بر اساس مدل سطح پاسخ ایجاد شده، از راه حل بهینه پارتو برای تعیین ترکیب بهینه پارامترهای عملیاتی آن استفاده شد: فشار مکش 26. مگاپاسکال، فشار خروجی اگزوز 0.45 مگاپاسکال و سرعت چرخش 2,099.80 دور در دقیقه. در نهایت، مدل عددی توسط بستر آزمایشی معاده شد: فشار مکش مقار خروجی ازمایشگاه سیستم مگاپاسکال، فشار خروجی اگزوز 20.5 مگایاسکال و سرعت چرخش 2,099.80 دور در دقیقه. در نهایت، مدل عددی توسط بستر آزمایشی ساخته شد. در آزمایشگاه سیستم مگاپاسکال، فشار خروجی اگزوز 20مای مگای مخته ارگانیک رانکین تأیید می هد. نتایج تعری مران می کند. تولید برق برون روغن حرارتی با دمای پایین جرعه ارای توسعه و اصلار ماشیزهای اسکرول آینده ارائه میکند.



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# Development of Temperature-strain Prediction Based on Deformation-induced Heating Mechanism in SCM440 Surface Cracked Shaft under Ultrasonic Excitation

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# PAPER INFO

# ABSTRACT

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The mechanisms behind temperature and material deformation in vibrothermography remain questionable, presenting a gap in understanding. This study investigates the deformation-induced mechanism, focusing solely on the heat generation associated with strain development. Both experimental and simulation approaches are incorporated. The experimental segment explores the temperature-strain relationship of SCM440 material, commonly used for rotating shafts. This behavior is examined through the connection between temperature change and material deformation during a uniaxial tensile test. Results indicate that temperature change and distribution can be predicted based on plastic strain development. Finite Element Method (FEM) simulation is utilized to model the excitation of a shaft with and without an elliptic surface crack. Various cracked shaft configurations are investigated, revealing distinct strain generation and distribution patterns. High strain alteration is notably observed around the crack tips, enabling the detection of shaft discontinuity. Consequently, a temperature prediction technique is developed to estimate temperature based on strain alteration during deformation. Adequate excitation power and the use of a high-sensitivity IR camera are recommended for the effective application of the temperature prediction technique. Additionally, this study provides insights into understanding the utility and limitations of vibrothermography for inspecting engineering component damage based on experimental temperature-strain relationships and computational predictions of strain distribution in cracked shafts under excitation. These findings offer guidance for engineering applications and future research endeavors.

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# **1. INTRODUCTION**

Vibrothermography (VT) is a technique to investigate the defect located on either the surface or near the surface via thermal energy release (1). This inspection technique requires an infrared (IR) camera to detect the diffused heat from vibrated defects. When the defects are vibrated, they rapidly generate heat that is diffused and radiated outward to the surface, which can be observed in a short time (2). Therefore, VT is less consumed in the inspection time compared with another nondestructive testing (NDT) technique, which is requisite for industrial interests. VT was first introduced in the late 80s by Reifsnider et al. (3). A series of experiments were conducted with noticeable heat generation in materials, and the thermographic pattern of heating depended on the material properties and structural geometry referred to by Reifsnider et al. (3) These indicated the unique characteristics of the thermal energy release on a specific material. Subsequently, VT became well-known after Favro et al. (4) placed an ultrasonic welder with a maximum power of 1 kW for the excitation source. Thereafter, an IR camera revealed the glow of a crack immediately after a sonic pulse was applied, which influenced more availability and reliability for industrial applications.

According to the industrial components, the metallic cylindrical-shaped component is a common part frequently involved in any system of the industry, i.e., axle, pin, shaft, etc. (5) Defects in these components are generally discovered as fatigue cracks, especially during the observation of shafts (6). In general, fatigue cracks are inevitable and normally appear in components that have operated repeatedly (7). A fatigue crack on a shaft can be initiated from a small discontinuity that occurs on the surface and transversely propagates to the center under cyclic loading conditions, which sequentially directs a large discontinuity and complete fracture (8-10). Recently, it has been observed that VT was applied for inspecting defects in industrial components, i.e. turbine disks, gas turbine blades, welded parts, etc. (11-14). The results revealed the good detectability of this inspection; VT could detect a known fatigue crack of 0.015 mm in length with a better possibility of detection (POD) than the traditional method (15). In addition, VT was capably performed on various materials such as concrete (16, 17), ceramics (18), polymers (19, 20), and metals (21-23). The aforementioned studies confirmed the usability, rapidity, and variety of this inspection method.

Vibroacoustic thermography (VT), also known as sonic IR and thermosonics, currently relies mainly on IR cameras and ultrasonic excitation. Ultrasonic excitation is typically selected at a predetermined frequency of 20, 40, or 60 kHz (24). However, the heating mechanism of VT remains questionable as it is not fully understood (14). It has been found that researchers attempted to investigate the source of heat generation. There are 2 major sources that have been discussed: (1) Frictional rubbing and (2) Deformation-induced heating (25). For instance, the severity of the closure crack rubbing during vibration can cause heat generation due to friction between the contracting faces of the crack. The evidence of frictional heating is shown in the following literature (26-28). Besides the closure crack, the asperity might be included, meaning no rubbing between crack faces. The heat can be induced beyond the crack tip due to the structural deformation under the vibration causing the stress concentration in the plastic zone, which is also known as plasticity-induced heating (29, 30). Nonetheless, deformation-induced heating in metal is rarely divulged due to the absence of demonstration. Therefore, the study of deformation-induced heating in metallic material is necessary for a better understanding of these heating mechanisms.

The understanding of material characteristics expedites the ability to estimate limitations or potential damage to engineering components within the system. In several instances, material characteristics have been employed to simulate their behavior under real working conditions or relevant scenarios in analytical models. The behavior of structures exhibits responses under assigned loading conditions, which aids in investigating structural deformations such as damage, elasticity, plasticity, and vibration (31-33). Analyzing these responses indicates the structural component usage experienced during operational conditions, allowing for the prediction of fatigue and service life (34-37). A similar approach is adopted to investigate temperature changes resulting from deformation-induced heating in this study. The developed temperature prediction technique demonstrates the object's temperature based on the corresponding strain alteration during deformation. This study aims to establish a fundamental understanding of the deformation-induced heating mechanism and to enhance the comprehension of the VT inspection technique used in engineering components excluding the frictional heating from closure cracks, serving as a foundation for future developments in industrial applications.

In this study, the temperature prediction technique was examined based on deformation-induced heating from the perspective of the vibrothermography inspection method. The study focused on the inspection of engineering parts that are widely used in industrial systems. The circular SCM440 shaft was selected for the study as it is commonly used for shafts in many applications (38). The study included both experimental and computational research. The experimental-based research was performed on the investigation of the temperature-strain relationship of the selected material for developing the prediction technique. Meanwhile, the computational research observed the response of the shaft under virtual ultrasonic excitation to investigate the influence of the controlling parameters including crack shape, crack size, and excitation conditions. This study attempted to determine the strain characteristics of the shafts, either with a crack or without a crack. The developed temperature prediction technique was applied afterward to estimate the temperature of the shaft based on the computed strain under ultrasonic excitation. The research methodology flowchart is illustrated in Figure 1.

# 2. EXPERIMENTAL INVESTIGATION OF THE TEMPERATURE-STRAIN RELATIONSHIP ON SCM440 MATERIAL

As reported by Reifsnider et al. (3), thermal characteristics are individually dependent on the material. To understand the behavior of temperature induced during structural deformation based on deformation-induced heating, the thermal characteristics of SCM440 (AISI 4140) due to structural deformation were investigated. From observation of previous experimental work conducted by Kapoor and Nemat-Nasser (39), the temperature (T) of an object during deformation can be described as Equation 1:

$$T = T_0 + \Delta T \tag{1}$$

where  $T_0$  is an initial temperature and  $\Delta T$  is the temperature change due to the deformation. In this work, the temperature change ( $\Delta T$ ) was investigated via the experiment with the following details.

**2. 1. Material Properties and Experimental Preparation** SCM440 steel was machined into flat tensile specimens according to ASTM E8 standard for uniaxial tensile testing and chemical composition, as



Figure 1. Research methodology flowchart

shown in Table 1. The inspection points on the specimen were selected to be in the gauge length and were marked as P1, P2, and P3. The P2 was in the middle of the specimen, while P1 and P3 were marked away from P2 with an equal spacing of 6 mm (see Figure 2). The influence of the surface preparation on the temperaturestrain relationship was included in this investigation. During the surface preparation process, the specimens were ground in different directions, denoted as the axial direction (Y-axis) and transverse direction (X-axis), as illustrated in Figure 2. Furthermore, the Pulstec µ-X360s was applied for X-Ray Diffraction (XRD) analysis. The cosine technique was performed with an incident angle of 35° to investigate the residual stress at marked locations. Lastly, the specimens were sprayed in a sparkle pattern to be ready for strain analysis using the GOM Digital Image Correlation (DIC) system.

**2.2. Procedure** A prepared specimen was attached with K-type thermocouples to the marked location and mounted on the universal testing machine. The thermocouples were connected to the NI-9213 temperature module for data logging. The sensitivity of the temperature-measuring module with K-type thermocouples was 0.02°C in resolution mode. An

 TABLE 1. Chemical composition of SCM440 material

 Element
 C
 Si
 Mn
 P
 S
 Cr
 Cn
 Ni
 Ma

Liement	C	01	14111	-	5	CI	Cu	1 11	1010
%Weight	0.41	0.23	0.78	0.16	0.13	1.06	0.02	0.01	0.17



Figure 2. Dimensions of ASTM E8 specimen with marked point



Figure 3. Experimental setup

extensometer and GOM ARAMIS adjustable camera were used for strain measurement where an extensometer griped across the specimen gauge and a GOM camera captured a deformation on the surface of the specimen, as shown in Figure 3. The tests were conducted at room temperature with 0.5 mm/min testing speed. A sampling rate was set at 1 Hz for all data logging. In the postprocess step, GOM Correlate software was applied to analyze the local strain at the location of the thermocouple attachment that constructed the temperature-strain relationship.

This temperature-strain relationship exposed the temperature of the SCM440 object via strain alteration. Comprehension of the temperature-strain relationship was utilized to explain the behavior of the cracked shaft on the strain response under excitation, which was investigated in the computational study.

# 3. COMPUTATIONAL STUDY OF SURFACE CRACKED AND UNCRACKED SHAFT ON STRAIN RESPONSE UNDER EXCITATION

In this session, VT was applied to a shaft, which is a common part of the rotating machinery in industry. Surface cracked and uncracked shafts were subjected to excitation using a low-power ultrasonic cleaning transducer. The application of a low-power ultrasonic cleaning transducer as an excitation source for VT has been previously published (40-42). Cracks can propagate when applied force exceeds the resistance of the material, resulting in the release of stored energy (43). Before crack propagation, the quasistatic energy was stored in a small region beyond the crack tip, known as the plastic zone. Considering the early stage of loading, the fracturecharacterizing parameter, i.e., the stress intensity factor (K), was used to define the stress fields. An example of the stress fields for the opening mode (Mode I) can be determined by Equation 2 (44):

$$\sigma^{(I)} = \frac{K_I}{\sqrt{2\pi r}} f^{(I)}(\theta) \tag{2}$$

where *r* denotes the distance from the tip and  $f(\theta)$  is the angular function that depends on the crack geometry and fracture mode; the mode of fracture was also based on the loading condition (43). From Equation 2, crack geometry and the condition of load governed the behavior of the stress fields near the tip.

The stress and strain relationship could be described by the material model. For metal and alloy, the strain ( $\varepsilon$ ) is usually directly proportional to stress ( $\sigma$ ) under elastic deformation, which obeys Hooke's law and could be expressed as Equation 3:

$$\varepsilon = \frac{\sigma}{E} \tag{3}$$

where E was the elastic modulus of the material.

The elastic strain around the crack tip is related to the loading condition and crack geometry. The effect of loading conditions and crack geometry were considered and investigated in this study. The finite element method (FEM) is a preferred method used for such analysis in the field of fracture mechanics. Several studies have utilized FEM to analyze the elastic-plastic response in various ways (45-50). In this study, ABAQUS FEA software was employed for the investigation of influences of crack geometry and loading conditions on the strain responses of both surface cracked and uncracked shafts.

**3. 1. Computational Model** This study aimed to investigate the strain response of a shaft under excitation using a low-power ultrasonic cleaning transducer. The initial step involved experimental calibration of the 40 kHz ultrasonic cleaning transducer in the laboratory. A 100 W signal generator was used to determine the force exerted during the transducer's operation, resulting in a force of 0.35 N. This force was applied as the excitation load (P) in the subsequent computational model. The computational model was created in ABAQUS FEA and represented a 3D cylindrical shape resembling both cracked and uncracked shafts. The dimensions of the shaft were derived from a drive shaft in a water pump system with measurements of 24 mm in diameter and 60 mm in length. The material chosen for the shaft was SCM440, a commonly used material for shaft applications. The stress-strain behavior of SCM440 was obtained through uniaxial tensile testing in the laboratory. The computational model employed implicitdynamic analysis to study the transient strain alteration under excitation. Note that, this study illustrated the methodology particularly on the adopted shaft geometry. The purposed methodology could later be extended without major difficulty to investigate other components with different geometry.

A simple cylindrical model was used to represent the uncracked shaft. For the cracked shaft, the contour integral technique, which is favored for studying the effect around the crack tip, was applied to create the crack. The elastic-plastic, power-law hardening material was adopted to control the strain singularity at the crack tips, which is commonly used for a stress-strain field analysis near the tips of elastoplastic materials (51-54). The cracks contained a crack front and crack faces, as illustrated in Figure 4. The crack tip that was located close to the angular displacement ( $\theta$ ) of 0 was denoted as CT1 and the far side was denoted as CT2. Interaction between crack faces was assigned as "Hard" in Abaqus nomenclature for normal behavior to prevent interferences. For tangential behavior, the coefficient of friction (COF) was selected arbitrarily at 0.8 according to the friction coefficient of steel on steel for dry contact conditions (COF = 0.5-0.8). However, the heat generated due to frictional rubbing and self-weight were not

considered in this work. The shaft model was small and subjected to vibrate at high frequency thereby the selfweight was considered negligible as the previous research (55). The uncracked shaft model was globally meshed with the C3D8R elements of 0.5 mm of mesh seed for the entire model. The curvature control factor of the mesh seed was set at 0.005 to increase the mesh density of the model which directly affected the accuracy of the finite element analysis result (56). The cracked shaft was modeled with the spider-web technique being applied to the area surrounding the crack with C3D20R and C3D15, which were quadratic elements to provide a precise result. The size of the element around the crack tip was nearly 0.005 mm to acquire a converged result. However, the rest of the models were applied with C3D8R to optimize the computational time. Furthermore, both areas had a different type of element and were tied with surface-to-surface constraints. An example of model meshing on shafts is shown in Figure 5.

# 3.2. Crack Characteristics and Loading Conditions

The transverse crack was one of the common cracks on a shaft that occurred frequently in a rotating shaft (57). In this study, the transverse crack was artificially created at the middle of the shaft length. The crack geometry was modeled based on a semi-elliptical crack shape with the crack length and shape factor serving as the controlled parameters. These parameters are illustrated in Figure 6. Characteristic length of crack ( $\alpha$ );

 $\alpha = a/R = 0.05, 0.1, 0.25, 0.5, 0.75, 1$ 



Figure 4. Isometric view of cracked shaft and cracked components



(a) Uncracked shaft (b) Cracked shaft Figure 5. Model meshing

Shape factor of crack ( $\beta$ );

 $\beta = a/C = 0$  (Straight crack front), 0.25, 0.5, 0.75, 1 (Circular crack front)

For the current study, the excitation directions and support conditions were varied to provide the different modes for the excited shaft. The modes of vibration depended on the direction of loading (58). The computational models consisted of two support conditions: cantilever support and fixed-end support. In the cantilever support configuration, the excitation load was applied on the free end of the shaft, referred to as axial excitation. In the fixed-end support configuration, the excitation load was applied transversely to the shaft at the middle, called transverse excitation, as shown in Figure 7. Furthermore, the diameter of the contact face for the ultrasonic transducer was measured at 45 mm.

# 4. TEMPERATURE-STRAIN RELATIONSHIP OF SCM440 AND TEMPERATURE PREDICTION

4. 1. Experimental Results of the Temperature-Strain Relationship The residual stress of the



Figure 6. Controlled parameters of the semi-elliptical crack



**Figure 7.** Excitation direction and boundary conditions on the cracked shaft; (a) Axial excitation with cantilever support, (b) Transverse excitation with fixed ends support

specimens is obtained as detailed in Table 2. The residual stress data provide a noticeable difference in the residual stress due to the different grinding directions under the surface preparation process. The larger compressive residual stress has been observed on the axis that is parallel to the direction of the grinding path. Under uniaxial tensile testing, the specimens that were ground similar to the loading direction are denoted as parallel ground and vice versa, denoted as perpendicular ground. The parallel ground specimens have slightly higher tensile stress than the perpendicular ground. The maximum difference of the ultimate tensile strength (UTS) between parallel ground and perpendicular ground specimens is approximately 40 MPa, which is less than 5%, indicating the negligible influence of the residual stress on the stress-strain curve. The average elastic modulus (E) and UTS of SCM440 steel are 201.4 GPa and 1080 MPa, respectively, as illustrated in Figure 8.

Temperatures have been observed under tensile testing, conveying the temperature increase during deformation. The temperatures increased corresponding to the strain of the tensile specimen. Considering the temperature before the necking, the temperature changes  $(\Delta T)$  of the parallel ground and perpendicular ground specimens have been plotted against the true equivalent strains (true  $\varepsilon_{eq}$ ) to investigate the influence of residual stress, as depicted in Figure 9. The average temperature changes were calculated individually for each case. The uncertainty of the temperature measurements on the parallel ground and perpendicular ground specimens was approximately ±0.2 °C, as shown in Figure 9a. The average temperature changes for both grinding specimens were compared to investigate the influence of residual stress, as shown in Figure 9b; the maximum difference of the temperature change between the parallel ground and perpendicular ground specimens was less than 0.07 °C. These results suggest that the residual stress had no significant influence on the temperature induced during deformation. Furthermore, the mean temperature change was calculated from the average temperature changes of both grinding conditions to describe the behavior of temperature during deformation.



Figure 8. Engineering stress-strain curve of SCM440 specimens



**Figure 9.** Temperature during deformation prior to necking, (a) Uncertainty of the temperature measurement, (b) Temperature variations under different grinding directions

<b>TABLE 2.</b> Residual stress at P1, P2, and P3	
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Grinding		Y-axis			X-axis		
direction	No.	<b>P1</b>	P2	P3	<b>P1</b>	P2	P3
	1	- 366.5	- 364.5	-371	- 134.5	- 137.5	- 132.5
	2	-362	-358	-364	-79	-88.5	- 102.5
Y-axis (Parallel)	3	-365	- 356.5	- 379.5	-134	- 103.5	- 116.5
	4	-384	- 373.5	- 357.5	- 102.5	- 103.5	-91
	5	-376	-370	- 356.5	- 126.5	- 139.5	-139
	6	-58.5	-60	-44.5	-361	-372	-364
X-axis (Perpendicular)	7	-122	-112	- 124.5	-352	-338	-347
	8	-56	-55	-44	-348	-383	-375
	9	-133	-106	-102	- 349.5	-351	- 351.5
	10	-49.5	-42.5	-59	- 372.5	-365	-359

From the observation, the behavior of the mean temperature change exhibits a relatively low-temperature change with a fluctuation in the beginning of elastic region and the temperature increases noticeably along the strain-hardening region, indicating the temperature changes substantially during plastic deformation.



Figure 10. Temperature-strain relationship

Furthermore, the mean temperature change is plotted against true equivalent strain prior to the necking, denoted as uniform equivalent strain ( $\varepsilon_{eq,uni}$ ), to construct the temperature-strain relationship, as demonstrated in Figure 10. The second degree of the polynomial curve fitting has good fit with the relationship curve, which has a confidence of  $R^2 = 0.9985$ . From curve fitting, the polynomial regression can be expressed as Equation 4:

$$\Delta T = -86.515\varepsilon_{eq,uni}^2 + 26.437\varepsilon_{eq,uni} - 0.0758 \tag{4}$$

4. 2. Prediction of Temperature Based on the **Temperature-Strain Relationship** The developed relationship was applied for the temperature prediction of the specimen under tensile testing. Similar material was machined into a standard tensile specimen with a circular cross-section of gauge diameter 6 mm and 25 mm long of gauge length, as shown in Figure 11a. These dog-bone specimens were painted in black to prevent reflection from ambient light. Moreover, an extensometer and FLIR A655sc infrared (IR) camera were also equipped in the test, as shown in Figure 11b. Non-Uniformity Correction (NUC) was set for the IR camera to automatically improve the temperature reading, which provided more accuracy during the record. The cross-head of the testing machine was set to 0.5 mm/min. The records were stopped after the specimen reached the necking stage to prevent accidental damage to the IR camera lens. Meanwhile, the computational model was additionally created to investigate the strain behavior during the test. The configurations were set accordingly to the constraints and boundary conditions of the experiment. As a result, the strain alteration of the tensile specimens obtained from the experiment and simulation are plotted to unveil the strain behavior during deformation, as observed in Figure 12. Under fixed-speed controlled deformation, the true strains of the tensile specimens have corresponding behavior, which barely changed under the elastic deformation and increased exponentially in the plastic deformation.

Regarding the temperature, the initial temperatures were measured prior to the test using an IR camera. The temperature behavior from the IR camera was investigated using ResearchIR software. The side-byside view between the temperature gradient and the distribution computational strain is displayed simultaneously in Figure 13a, which reveals a comparable color contour. Hence, the strains were sequentially substituted into Equation 4 and Equation 1 for determining the predicted temperatures. The predicted temperatures were plotted to compare with Figure 13b demonstrates a significant correlation between the temperature predictions and the actual temperature during deformation. The accuracy of these predictions is detailed in Table 3. The maximum absolute error observed among the multiple tests was approximately 0.4 °C, which suggests a close agreement. These findings suggest the potential usability of the temperature-strain developed relationship for temperature prediction based on strain alteration with a disagreement of less than 1.5%. The results provide compelling evidence that the deformation temperature can be estimated effectively when the corresponding strain alteration is known. It is important to note that the developed relationship is specifically applicable to SCM440 material with a constant deformation speed of 0.5 mm/min.



Figure 11. Experimental temperature prediction setup



**Figure 12.** Strain alteration prior to necking the actual temperature within the gauge section, as presented in Figure 13b



Figure 13. Temperature prediction, (a) Temperature and strain distribution at t = 630 s, (b) Comparison of temperature predictions

**TABLE 3.** Accuracy of temperature prediction under uniaxial tensile testing

		Maximum error				
No.	Initial temperature (°C)	Absolu	ute (°C)	Percentage (%)		
		EXP.	FEM.	EXP.	FEM.	
1	26.405	0.220	0.218	0.785	0.829	
2	26.533	0.409	0.384	1.489	1.436	
3	26.442	0.311	0.370	1.132	1.382	

# 5. STRAIN RESPONSE OF THE CRACKED AND UNCRACKED SHAFT UNDER EXCITATION

5. 1. Computational Investigation of Uncracked Shaft The computational results show the response of the stress field generated under excitation. Stress is generated following the deformation of the vibrated shaft. The shafts vibrate back and forth in different directions depending on the excitation direction. For example, axial vibration occurs under the axial excitation condition and transverse vibration occurs under the transverse excitation condition. Under the investigations, stresses were found within the yield limit, which could be directly converted into the corresponding strains using Hook's law (Equation 3). The behavior of stress distributions varies between the two excitation conditions due to the dissimilarity of the stress propagation. Under axial excitation, stress propagates along the length of the shaft, creating a longitudinal stress distribution. In contrast, stress is distributed from the top to the bottom

of the shaft under transverse excitation, resulting in lateral stress distribution. These observations are displayed in Figure 14, which shows the distinct patterns of strain contour under each excitation condition. At the middle of the shaft where the stress is fluently distributed under both excitations, strain responses are observed, as shown in Figure 15a, which reveals the dynamic behavior of strain. The response between both excitations shows slight phase shifting and varying amplitudes. Examining the first peak of the responses that display close characteristics, the circumferential surface strains under both excitations are plotted to display the strain distribution, as depicted in Figure 15b. Under axial excitation, the strain distribution is uniform along the shaft circumference. On the contrary, the strain under transverse excitation exhibits a distinct pattern.

It is the highest at an angular displacement ( $\theta$ ) of 0, where excitation takes place and reaches its lowest at  $\theta =$  $\pi/2$ . Then, the strain increases gradually as the angular displacement progresses towards  $\theta = \pi$ . This finding highlights the significant influence of the excitation source on strain generation in the excited shaft under transverse excitation, particularly in the vicinity of the excitation location. The excitation source plays a notable role in elevating strain levels, and it is crucial to recognize the influence of the excitation source on strain generation during analytic consideration. In this study, the strains at the opposite side of the excitation ( $\theta = \pi$ ) for transverse excitation are considered to minimize the direct influence of the excitation source on the strain measurement. From the observation, the maximum strain generations due to the deformation under the excitations of uncracked shafts were found to be 3.89x10-9 and 4.72x10<sup>-9</sup> for the axial and transverse excitation, respectively.

**5. 2. Experimental Investigation of Uncracked Shaft** This section explains the experiments conducted to observe the deformation of the uncracked shaft under



**Figure 14.** Top view of the strain distribution on the uncracked shaft under excitation, (a) Axial excitation, (b) Transverse excitation



**Figure 15.** Strain responses of the uncracked shaft at the middle, (a) Example of the strain response at  $\theta = \pi$  (b) Circumferential strain under excitations

excitation. For instance, in the case of the transverse excitation, the jig and fixture were designed to securely hold the uncracked shaft in fixed-ends support condition, as shown in Figure 16. An ultrasonic transducer was positioned on the slider body of the linear guide rail, which was utilized to minimize the influence of gravitational force and apply excitation to the side of the shaft. The slider body was connected to an adjustable pin, and a helical spring was incorporated to allow for the adjustment of contact pressure between the transducer and the shaft. The contact pressure can be calculated based on the compressive length and stiffness of the spring, which was determined to be 2.8 N/mm under the compression test. The designed jig and fixture were clamped securely onto a rigid table, with a rubber plate placed in between to isolate the system from the surrounding environment. To measure the deformation on the surface of the shaft during excitation, a 3D digital image correlation (DIC) system was utilized. The system was set to record real-time data at a maximum resolution of 40 frames per second. Before conducting the test, an SCM440 shaft with a diameter similar to the one used in the computational study was prepared by spraying a pattern for surface mapping and marking a reference point for precise analysis. Meanwhile, the computational model used in this section was modified to match the experimental setup. An initial load was applied to simulate the preloading caused by the contact pressure of the ultrasonic transducer. The load was offset by 19.7 N, corresponding to a 7 mm compression of the spring in the experimental setup. However, the other configurations remained the same as in the previous setups.



Figure 16. Experimental setup for validation of the computational results



**Figure 17.** Digital image-processing using GOM correlation software, (a) Images captured by the GOM DIC system (b) Quality and angular displacement of the surface mapping

Under the investigation, the magnitudes of deformation on the shaft surface were observed in the response during excitation. For the experimental data, the different angles of the excited shaft were captured using the dual camera setup on the DIC system, as displayed in Figure 17a. Both images were used to construct a 3D surface model based on the prepared surface pattern, thus facilitating the measurement of surface changes. The shaft surface pattern was mapped using the GOM correction software for digital image processing. The surface mapping captured approximately 144° of angular displacement. The quality of the mapping was examined and rated on a scale from 0 to 10, with 10 indicating high quality and 0 indicating poor quality. The results indicated that the mapping exhibited high quality around the front part of the shaft, as illustrated in Figure 17(b). Furthermore, the magnitude of deformation was normalized with respect to the reference point located in the middle of the shaft.

When comparing the results, the steady state was considered where the response exhibited a consistent behavior. Figure 18 displays the contour of the magnitude of deformation from both experimental and computational investigations, revealing the similar behavior of the shaft. A significant deformation was observed in the middle region, which gradually decreased toward the fixed ends. The experimental investigation showed slightly higher deformation around the fixed-end supports compared to the computation, indicating a small translation motion of the designed fixture during excitation. Additionally, the magnitude of deformation along the circumference at the middle of the shaft was also investigated, as depicted in Figure 19. The experimental results showed a slight difference compared to the computational results, particularly in the vicinity of the excitation source. The magnitude of deformation observed in the experiment was higher than what was predicted by computation. The difference could be attributed to several factors, including potential issues with surface mapping quality at the edge of the shaft or the presence of a non-rigid fixture at the fixed ends. The percentage error prior to the angular displacement of  $\pi/4$ was up to 10%. Nevertheless, the percentage error beyond the angular displacement of  $\pi/4$  was less than 5%, indicating good agreement with the computational results beyond the angular displacement of  $\pi/4$ . Besides, both responses demonstrated similar behavior, exhibiting consistent patterns of deformation with high magnitudes of deformation near the excitation source and lower magnitudes on the opposite side. Based on the comparison of the shaft response in both investigations, the behaviors exhibited by the shaft under excitations are well-correlated, particularly in the middle region and the farther region of excitation. These findings strongly support the effectiveness of the current configurations of



**Figure 18.** Deformation magnitude of the uncracked shaft under transverse excitation, (a) Experiment, (b) FEM



Figure 19. Comparison of deformation magnitude along the shaft circumference

the computational model for studying the shaft response under excitation.

Working under low-power excitation, especially for ultrasonic applications, is challenging because of the sensitivity and rapidity. Accurate measurement of alterations requires the use of highly responsive equipment with high sensitivity. In this experiment, the intention was to employ an infrared (IR) camera with a developed temperature prediction technique for temperature measurement.

However, the strain responses of the uncracked shaft under the excitations studied indicated that the technique was not yet fully applicable. The computational investigation revealed extremely low strain responses under excitations significantly below the yield point. Additionally, the DIC system could not accurately capture these low-strain alterations due to its limitations. The strain contour of the excited shaft under the computational investigation is displayed in Figure 20, including temperature prediction using the temperaturestrain relationship, assuming a constant initial temperature of 25 °C. The predicted temperature was observed to be approximately  $24.92^{\circ}C \pm 0.0001\%$ . The maximum temperature difference was much less than the thermal sensitivity of the currently used IR camera (0.03 °C). Temperature changes were unnoticeable on the IR camera, as expected. The results indicated that the excitation power applied by the low-power ultrasonic cleaning transducer was insufficient, implying the need for the enhancement of excitation power to summarize the changes in practical measurement.

The temperature prediction technique based on strain alteration is likely to be applicable for deformation detection. However, the temperature of the uncracked shaft under excitation was well below the sensitivity threshold of the IR camera, resulting in undetectable changes. Nevertheless, the developed temperature prediction technique has the potential to be effective in estimating the temperature changes when utilized with a high-sensitivity IR camera and accurate predictions of the deformation are available. Hence, the study aims to investigate the strain response on the cracked shaft. The computational model of the uncracked shaft is extended, including a surface crack at the middle of the shaft.



Figure 20. Temperature prediction of the uncracked shaft under the transverse excitation

# 5. 3. Extended Model for Investigation of Cracked

Shaft During the investigation of the extended model for the cracked shaft, plasticity was not observed. The stresses under excitation remain within the yield limit of the material. Figure 21 displays the strain distribution under axial and transverse excitations, revealing a slightly different contour from the previous investigation of the uncracked shaft due to the meshing adjustment in the outside crack area to optimize computational time. For the vicinity of the middle region where the crack is located, the strain is mainly concentrated around the crack tips, where it is noticeably higher compared to the uncracked shaft. However, no crack propagation was observed. Considering the behavior of the strain around the crack tips under the stress flow due to excitation, the localized strains at both tips of the crack are simultaneously equivalent under the axial excitation. In contrast, strains under the transverse excitation exhibit time-dependent variations in strain generation at the crack tips. The strain generation at the crack tip oscillates over time showing periodic pattern, with higher strain observed initially at the tip closer to the excitation and then gradually reduced with higher strain being observed at the tip located farther away from the excitation. The crack tip at the far side of the excitation (CT2) is selected for the investigation of strain generation to minimize the influence of the excitation source, which was previously found in the investigation of the uncracked shaft under the excitation. The strain generation at the tip of the cracked shaft is significantly higher than the maximum strain generation of the uncracked shaft. The strains are normalized with the maximum strain observed in the uncracked shaft. Sequentially, the normalized strains are plotted against the characteristic parameters of the crack under various excitation conditions aiming to investigate the influence of the crack geometry on strain alteration at the crack tips. The results of the analysis are presented in Figure 22.

Figure 22 illustrates the influence of crack geometry on the strain alteration surrounding the crack tip. Larger cracks result in a higher strain, as demonstrated by a circular crack with a characteristic length of 0.75 ( $\beta = 1$ ,



**Figure 21.** Example of the strain distribution on the cracked shaft under excitation, (a) Axial excitation on the circular cracked shaft ( $\beta = 1$ ) with  $\alpha = 0.5$  (b) Transverse excitation on the circular cracked shaft ( $\beta = 1$ ) with  $\alpha = 0.5$ 



**Figure 22.** Influence of the crack geometry on strain alteration beyond the crack tip, (a) Axial excitation, (b) Transverse excitation

 $\alpha = 0.75$ ) exhibiting greater strain alteration compared to a circular crack with a characteristic length of 0.5 ( $\beta = 1$ ,  $\alpha = 0.5$ ) under excitation. Besides, the circular crack front  $(\beta = 1)$  demonstrates the highest strain during excitation, while the straight front ( $\beta = 0$ ) exhibits the lowest strain under observation. This behavior consistently shows a similar pattern, except for the straight front crack with  $\alpha$ = 1 under transverse excitation. The strain of the straight front crack is noticeably higher than the crack with  $\beta$  = 0.5 at a similar characteristic length of  $\alpha = 1$ . To understand the disparity, a comprehensive analysis was carried out by plotting the strain alteration over time for all examined crack geometries with  $\alpha = 1$  under the transverse excitation. Figure 23a reveals the extreme shift of phases on the straight front crack ( $\beta = 0$ ), while the other crack fronts ( $\beta = 0.25$  to 1) exhibit a slight shift of phases in the response. The reason for the massive phase shifting of the straight front crack ( $\beta = 0$ ) shaft under the transverse excitation may arise from the alignment of the crack with the excitation direction. One of the tips of this crack configuration ( $\beta = 0, \alpha = 1$ ) locates directly under the excitation source, causing the load to transfer through the crack front to the other tip where the measurements are taken. Figure 23b illustrates the layout of the crack shaft, which contains a straight front with  $\alpha = 1$  under transverse excitation. The crack is aligned in line with the excitation direction, which could be the major cause of the phase shifting that leads to the difference in the strain behavior of the straight front crack ( $\beta = 0$ ) with  $\alpha = 1$ under transverse excitation, highlighting the alignment of the excitation source must be considered in the analysis for estimation purpose. Overall, the crack geometry of the circular cracked shaft influenced the alteration in strain surrounding the crack tip, which increased with the shape factor ( $\beta$ ) and the characteristic length ( $\alpha$ ). These findings align with prior research involving surface semielliptical cracked shafts. For instance, Carpinteri, A. unveiled the relationship between the geometry correction factor (FI) and the characteristic length of the stress intensity factor in the circular cracked shaft under cyclic axial loading (59). The geometry factor of the opening mode stress intensity factor for a surface crack in the solid cylinder can be expressed as Equation 5 (60):

$$F_I = \frac{K_I}{\sigma \sqrt{\pi a}}; F_I \propto \frac{1}{\sigma}$$
(5)

where the coefficient 'a' represented the crack depth. The relationship between the geometry factor and the characteristic length revealed a lower geometry factor with an increasing shape factor as depicted in Figure 24. Comparing this relationship with the strain alteration and characteristic length relationship found in the current study, it shows that the behavior of strain corresponds with Carpinteri's work. Since the lower geometry factor indicated the higher stress as it was inversely proportional according to Equation 5 and stress was directly proportional to strain within the elastic which was also found in the cracked shaft responses of this analysis. These findings indicate that strain alteration was higher with the increasing shape factor, similar to the findings of the current study as discussed. Other studies have shown similar results of the geometry factor and the characteristic length relationship as following literature (60-63).

In addition, the temperature prediction technique is applied to estimate the temperature from the strain of the excited cracked shaft to illustrate the surface temperature prediction. The technique is performed on the cracked shaft with a circular front and a characteristic length of 1 ( $\beta = 1$ ,  $\alpha = 1$ ), which has been observed as the crack geometry generating the highest strain under both excitation conditions. Figure 25 displays the strain contour with the predicted corresponding temperature.



**Figure 23.** Responses of the cracks with  $\alpha = 1$  under transverse excitation, (a) Strain responses of the different crack front (b) Section view of the straight front crack under excitation



**Figure 24.** Geometry correction factor variation near crack tips along the crack characteristic



**Figure 25.** Strain contour and predicted corresponding temperature, (a) Axial excitation of the circular cracked shaft ( $\beta = 1$ ) with  $\alpha = 1$ , (b) Transverse excitation of the circular cracked shaft ( $\beta = 1$ ) with  $\alpha = 1$ 

The maximum temperature differences are  $1.67 \times 10^{-5}$  °C and  $1.46 \times 10^{-5}$  °C for axial and transverse excitation, respectively. The temperature differences show a significant increase compared to the predicted temperatures of the maximum strain on the uncracked shaft ( $1.03 \times 10^{-7}$  °C for axial excitation and  $1.25 \times 10^{-7}$  °C for transverse excitation), with percentage increments of  $1.63 \times 10^{4}$  % and  $1.17 \times 10^{4}$  %, respectively.

Despite the increment, the temperature changes in the cracked shaft are still hardly measurable in practice, emphasizing the insufficient excitation power from the currently used ultrasonic transducer.

The improvement of excitation power and the use of a high-sensitivity IR camera are strongly recommended to enhance the effectiveness of the temperature prediction technique in practical applications. Estimating the defective area is achievable by leveraging the strain distribution around the crack through the utilization of an IR camera to capture the corresponding temperature .

It's crucial to emphasize that the temperature prediction technique was developed within a controlled environment in a research laboratory. Temperature variations can potentially influence material stiffness and heat transfer (64). While conducting, the impact of the ambient conditions, especially the surrounding temperature, should be taken into account. Consequently, the technique may not be well-suited for use in hotworking conditions, where significant changes in material properties occur and are affected by thermal radiation from surrounding components. In such conditions, both of the temperature detectability and the prediction accuracy may be compromised.

In contrast, the technique appears more suitable for natural ambient conditions, where temperature fluctuations are relatively modest compared to the extreme conditions of the hot-working conditions. Nevertheless, it's essential to acknowledge that even in natural ambient conditions, the external variables like sunlight and wind can influence temperature-induced changes, affecting the accuracy of temperature predictions.

For a comprehensive understanding, further studies should be undertaken to improve this technique and observe its limitations in real-world inspection scenarios.

# 6. CONCLUSION

This study carried out observations on the deformationinduced heating mechanism of SCM440 material. The observations revealed a correlation between temperature and deformation strain, where the temperature increases along the strain alteration. The results of the study suggest that the temperature can be predicted from the strain using the temperature-strain relationship. The developed temperature prediction technique can be applied to estimate the temperature of tensile specimens, demonstrating good predictability with a maximum absolute error of approximately 0.4 °C among multiple tests. Moreover, computational-based studies were involved in this work. Both cracked and uncracked SCM440 shafts were investigated for strain responses under ultrasonic excitation. The computational model was tested under different control variables, including

crack shapes, sizes, supports, and excitation conditions to investigate their influence on the strain responses. The experimental validation exhibited good agreement for the computational model with the shaft response under excitation. The results for the cracked shaft revealed significantly higher strain responses compared to the uncracked shaft, with the circular front crack exhibiting the greatest strain generation under any excitation conditions. The temperature prediction technique was also applied to estimate the temperature gradient from the strain distribution of shaft responses. However, the strain responses under the studies were very small with an excitation force of 0.35 N generated by the low-power ultrasonic cleaning transducer employed in this work, resulting in undetectable temperature changes in practice. To effectively utilize this prediction technique, improvements in the excitation power and the use of a high-sensitivity IR camera are required. Based on both investigations, the results strongly suggest that the temperature prediction technique can effectively estimate defective areas due to the strain distribution around a crack. Further studies should be conducted to optimize the temperature prediction based on the strain alteration technique for practical applications.

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#### Persian Abstract

# چکیدہ

مکانیسمهای پشت تغییر شکل دما و مواد در ویبروترموگرافی همچنان مشکوک هستند و شکافی در درک ایجاد میکند. این مطالعه مکانیسم ناشی از تغییر شکل را بررسی میکند و تنها بر تولید گرما مرتبط با توسعه کرنش تمرکز میکند. هر دو روش تجربی و شبیه سازی گنجانیده شده است. بخش تجربی رابطه دما-کرنش ماده SCM440 را که معمولاً برای شفتهای چرخشی استفاده میشود، بررسی میکند. این رفتار از طریق ارتباط بین تغییر دما و تغییر شکل ماده در طول آزمایش کشش تک محوری بررسی میشود. نتایج نشان می دهد که تغییر دما و توزیع را می توان بر اساس توسعه کرنش پلاستیک پیش بینی کرد. شبیهسازی روش المان محدود (FEM) برای مدلسازی برانگیختگی شفت با و بدون ترک سطحی بیضوی استفاده میشود. پیکربندیهای مختلف شفت ترک خورده بررسی میشوند و الگوهای تولید و توزیع کرنش متمایز را آشکار میکند. تغییر شفت با و بدون ترک سطحی بیضوی استفاده میشود. پیکربندیهای مختلف شفت ترک خورده بررسی میشوند و الگوهای تولید و توزیع کرنش متمایز را آشکار میکند. تغییر نقت با و بدون ترک سطحی بیضوی استفاده میشود. پیکربندیهای مختلف شفت ترک خورده بررسی میشوند و الگوهای تولید و توزیع کرنش متایز را آشکار میکند. تغییر دم بالا به طور قابل توجهی در اطراف نوک ترک مشاهده می شود که امکان تشخیص ناپیوستگی شفت را فراهم می کند. در نتیجه، یک تکنیک پیشینی دما برای تخمین دم بر اساس تغییر کرنش در طول تغییر شکل توسعه داده میشود. قدرت تحریک کافی و استفاده از دوربین IR با حساسیت بالا برای کاربرد موثر تکنیک پیشینی دما توصیه میشود. علاوه بر این، این مطالعه بینشهایی را در مورد درک کاربرد و محدودیتهای لرزش گرموگرافی برای بازرسی آسیب اجزای مهندسی و تلاشهای تعییر دما حرانش میشود. علاوه بر این، این مطالعه بینشهایی را در مورد درک کاربرد و محدودیتهای لرزش گرموگرافی برای بازرسی آسیب اجزای مهندسی و تلاشهای تعیقاتی آینده ارانه میکند.



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# Investigation of Antifouling Paints for Vessel in Tropical Seawater of North Jakarta in Indonesia

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# ABSTRACT

The copper-based biocide is mostly used as primary additive of Antifouling (AF) paint in Indonesia especially on vessels. The evaluation for the efficacy of AF paint was conducted where anti corrosion (AC) paint was also as a reference. The panels with both paints were exposed to various sea depths of up to 3 meters until 12 months of exposures. The measurement of parameters of seawater consisting of water conductivity, pH, temperature, dissolved oxygen and salinity were carried out. There was no or less attached marine biofouling on AF-painted panels but not on AC-painted panels up to 12-months of field exposure in various sea depths. There was no difference between the properties of AF paints before and after exposure to various sea depths. The inhibitive performance of AF paint depends on the existence of AF layer containing Cu<sub>2</sub>O biocide where the thickness of that layer decreases in increase of time exposure.

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# **1. INTRODUCTION**

The existence of marine biofouling have potency of major issues for the physical and mechanical degradation of submerged offshore structures particularly metal and alloys (1). The growth and settlement of biofouling have a detrimental effect on submerged structure (2-4). The metabolism of biofouling organisms may cause a decrease in corrosion resistance, an increase in drag, and a reduction in the frequency of drydocking operations for ships (5-8). The presence of corrosion could induce mechanical properties and operational time on existing structures (9, 10). In addition, the safety issues have been taken an essential part of consideration when the decrease of structure stability due to the growth and settlement of marine biofouling (11, 12). The biological metabolism of marine biofouling is mainly affected by seawater factors such as salinity, pH, water flow, dissolved oxygen, water temperature and surface

aggressively as a result of the warmer seawater temperature and higher salinity in tropical zones compared to those in temperate zones. Indonesia is one of several tropical countries with a hot and humid climate. Due to the warm surface water temperature and high salinity in the marine environment, the seasonal change is comparatively consistent every year. Additionally, Indonesia's ocean waters are home to a variety of marine species and ecosystems in both deep water and along the coast. Therefore, in Indonesia, marine biofouling continues to grow and settle without interruption, but not in subtropical countries. The usage of antifouling (AF) paint on marine submerged structures is a frequent mitigation strategy for the severity of associated marine biofouling. Biocide is typically the added chemical that makes up the majority of AF paints. The biocide of copper (Cu<sup>2+</sup>) being released from the

temperature (13, 14). Furthermore, the increased growth rate of biofouling organisms frequently occurs

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bulk of AF paint has the advantage of preventing biofouling from adhering to the structure (3).

Moreover, the poisonous property of copper compounds serves to inhibit the growth of some microand macroorganisms, including mollusks, algae, bacteria, and other organisms (15, 16). The usage of AF paint is the most proven method of mitigation up to now (17). Commonly AF paints comprise three types such as hard AF paint, ablative AF paint and self-polishing copolymer (SPC) AF paint. In Indonesia, SPC-AF paint is used at ship and boat due to the longer operational time service compared to other AF paints for the last 15 years. In addition, the other justification for using SPC-AF paint is the improved management of the discharge of copper compound or cuprous oxide (Cu<sub>2</sub>O), which act as the primary biocides (12). Due to the negative impacts of tributyltin (TBT) compound as prior biocides, tin-free self-polishing copolymers (tin-free SPC) AF paint has now been used as AF paint incorporating copper biocide. Generally, generic SPC-AF paint comprises resin, solvent, pigment, biocide, co-biocide, anti-settling agent, extender and soon on.

In preceding investigation, few researchers had reported the efficacy of SPC-AF paint in North Jakarta and Madura strait, Indonesia within a month after field exposure (4, 18). However, there is no comprehensive investigation the efficacy of SPC-AF paint perfomance for a longer exposure in Indonesia in North Jakarta especially the relationship amongs the depth of seawater level, intrinsic properties of SPC-AF and seawater parameters againts tropical marine biofouling particulary a binder of silyl acrylate. Therefore, this research aims to clarify the effectiveness of performance on SPC-AF paint compared to anticorrosion paint as reference material for a longer exposure up to 12 months in North Coastal of Jakarta District, Indonesia.

# 2. MATERIALS AND METHODS

2. 1. The Preparation of Specimens A plate of low carbon steel was cut (length: 25 cm, width: 20 cm and thickness: 0.03 cm) for a coating metal substrate. By using a portable sandblaster, all metal substrates were sanded in accordance with ISO 8501-1 Sa 2.5. According to that ISO standard, stains, streaks, and rust should only cover 5% of the steel substrate's surface. In addition, SPC-AF paints is classified as a top coat which define as a final layer of multiple paint layers over intermediate layer and primer layer. SPC-AF paints are essentially a three-layer system made up of an epoxy primer base coat, an epoxy intermediate base coat, and an epoxy top coat. There were two commercial SPC-AF paints used in this current work (AFP-A and AFP-B). On other hand, as controlled paint, anticorrosion (AC) paint also was applied over epoxy primer coating. In addition, both AF paints were received from two distinct Indonesian companies that specialize in tin-free self-polishing copolymers (SPC). Those companies produced the generic type of AF paint using the certain chemical formulas as well as that in preceeding work (19).

In early September, during the tropical rainy season, each test rack of both samples of AF paint and AC paint was positioned on submerged piles of Muara Baru sea port in North Jakarta (6°05'46.0"S 106°48'01.0"E), as shown in Figure 1. In addition, Geographically, Jakarta is located in an alluvial plain that is low and flat, with an average elevation of 8 meters (26 feet) above sea level with historically large swampy areas. North Jakarta region is a suitable field area to represent the environmental parameters and the growth of tropical biological fouling. In this field work, the exposure time was carried out by 2, 3, 6 and 12 months. In addition, during operational times, the maximum lifespan of SPC-AF paints is approximately 36 months where the recent evaluation of those paints efficacy was conducted before that lifespan. The evaluation of potential damage to those paints before the maximum operational time is needed in this work, especially in tropical countries like Indonesia. Following a period of exposure, the specimen was retrieved from the water and kept in storage until further characterization and analytical steps, as shown in Figure 2.

Furthermore, the settlement of marine biofouling on structure is affected by the water parameters such as water conductivity, salinity, pH, water temperature and dissolved oxygen (1, 4, 18). Those water parameters could be considered to be carried out in this present work where were measured by using HACH HQ40d Advanced Portable meter during operational service.

**2. 2. Evaluation of AF Paint Properties** In this work, paint testing was conducted to evaluate physical and mechanical properties of paints before and after field test. Paint was tested for hardness using the Elcometer 501 pencil hardness tester in accordance with American Standard Testing and Material (ASTM) D-3363. The evaluation pencil hardness was valued through the ranges



Figure 1. Location of specimen placement in Muara Baru, Jakarta, Indonesia



Figure 2. An activity of paint specimen retrievement at certain time of exposure in Muara Baru Sea port, North Coastal of Jakarta

from 6B (softest) up to 9H (hardest). The adhesion strength of paint was carried out using Elcometer 510 Automatic Pull-Off Adhesion Gauge according to ASTM D-4541. Adhesive strength refers to the ability of a paint to stick to surface of metal subtract and bond two surfaces together. Horiba Gloss Checker IG-331 was also used to perform properties of glossy at a 60-degree angle (ASTM D-523). In order to maintain the accuracy of the results, the tests were also run five times. The specimens are visually examined to check for the presence and distribution of biofouling. A JEOL JSM-6390 series scanning electron microscope was used to observe the cross-sectional morphology of samples.

# **3.RESULTS AND DISCUSSION**

3. 1. The Paint Properties and Seawater **Parameters after Exposure** The gloss properties of AFP-A and AFP-B following field exposure in various depths of saltwater are shown in Figures 3, respectively. The value of AFP-A and AFP-B gloss are 7.0 and 3.0 in the field test before exposure, respectively. The cause of gloss values difference in both AF paints is due to the lesser solid content of Paint A compared to Paint B. On the basis of result, the magnitudes of AFP-A gloss were almost the same each exposure time as well as those of AFP-B gloss. Low gloss AF paint is defined as having values of less than 10 Gross Units (GU), which were achieved by both AF paints. On the basis of results, the magnitudes of gloss paint are almost the same in both certain exposure times and different sea depths. It was found that both AFP-A and AFP-B had nearly the same gloss properties both before and after exposure.

Furthermore, both AFP-A and AFP-B are classified as tin-free self-polishing copolymers that have self polishing mechanism in paint matrix during service in marine environment. That mechanism can make surface of AF paint smooth until no more outer AF coating layer



**Figure 3.** (a) Glossiness of the AFP-A as a function of sea depth and (b) Glossiness of the AFP-B as a function of sea depth

on primary coating during service (19). In addition, the roughness of paint surface is attributed with gloss degree of coating (20). Before and after field exposure, the pencil hardness values of both AFP-A and AFP-B were classified in B scale. In addition, during field exposure, the pencil hardness values of AFP-A and AFP-B are the same.

Figure 4 shows that adhesion strength for AFP-A and AFP-B as function of depth levels of the sea after exposure. In varying levels of sea depth, the adhesion strengths of the paints were almost the same. There is no significant alteration of adhesion strengths in both two type of antifouling paints in different sea depth. The category of coating failures refers to 100% cohesion pattern, where both AFP-A and AFP-B occurred failure in a layer of antifouling coating as shown in Figure 5. Cohesive failure is in the coating itself due to internal crack (21) where that crack caused by abrasion process and dissolving additive in coating matrix. Main factors include water temperature, salinity, pH, dissolved oxygen, and others cause biological fouling to settle (19, 22). Most marine biofouling organisms suitably grow and settle in the environment with pH 7.5-8.0 and temperature of more than 20oC (23). Furthermore, North Jakarta bay is distinguished by its shallow water, 13 rivers flowing into it, and connections to the Java Sea which has been impacted by tropical seawater parameters. On the basis of results, the temperatures and pH of

seawater has the appropriate growth and settlement for marine organism where there are no or less shift alteration for those parameters in various depths of sea and different exposure times as shown in Table 1.

The dissolved salt concentration of bodily water is referred to as salinity, and the typical average saltwater salinity is around 35 ppt (24). The Muara Baru area of Jakarta Bay has salinity levels less than 35 ppt. North coastal of Jakarta has many estuaries near coastline which is lower salinity value in the range of 24-33.5 ppt (25) as well as the present results. Furthermore, the solubility of dissolved oxygen (DO) commonly increases in decreasing water temperature and vice versa (26) where DO concentration decreased with increasing seawater depth (27).





**Figure 4.** Adhesion strength for (a). AFP-A and (b). AFP-B as function of depth levels of the sea after exposure



Figure 5. An illustration of AF paint adhesion failure after exposure

Exposure time (months)	Depth (meter)	Temperature (°C)	рН	Salinity (ppt)	DO (mg/L)	Conductivity (mS/cm)
	0	30.9	8.2	28.1	5.58	48.7
2	1	30.7	8.3	28.2	5.44	48.7
2	2	30.6	8.3	28.2	5.2	48.6
	3	30.6	8.3	28.1	5.25	48.5
	0	30.45	8.35	28.15	5.06	48.45
2	1	30.35	8.38	28.15	4.937	48.38
5	2	30.25	8.41	28.15	4.814	48.31
	3	30.15	8.44	28.15	4.691	48.24
	0	30.05	8.47	28.15	4.568	48.17
E	1	29.95	8.5	28.15	4.445	48.1
6	2	29.85	8.53	28.15	4.322	48.03
	3	29.75	8.56	28.15	4.199	47.96
	0	30.7	7.79	29.9	1.89	51.4
12	1	30.7	7.79	30.1	1.6	51.7
12	2	30.7	7.8	30.5	1.05	52.4
	3	30.7	7.81	31.1	0.03	53.3

**TABLE 1.** Seawater parameter during field exposure at Muara Baru, North Jakarta

The level of DO is practically the same concentration at different depths below sea level up to a depth of three meters. The lowest magnitude of DO took place in 12 months of exposure. The authors presume that the significant decrease of DO concentration each depth of sea is caused by anthropogenic activity nearby Muara Baru, North Jakarta in 12 months of exposure. In addition, the euphotic zone is defined as the area with a maximum sea depth of 3 meters as well as this work. The penetration of the radiation of sunlight occurs intensively (27) where the active photosynthesis process supplies oxygen level in water (28). Moreover, Table 1 presents that water conductivity is nearly the same magnitude at different sea depths. Sea water commonly has average conductivity of approximately 55 mS/cm (29). However, in the present results, the values of conductivity each interval exposure is lower than 55 mS/cm.

When considering the effectiveness of antifouling paint, temperature, pH variations, DO and saltwater salinity are all essential factors. The solubility of biocides took place in small changes in the alkaline behavior of seawater, whether due to the production of hydrosulfide (pH decrease) or an increase in pH due to a decrease in  $CO_2$  caused by the presence of algae. The effectiveness of antifouling paint is constrained by the rate of chemical and enzymatic reactions, which accelerate the slow stages of cell growth and the rate of polymeric coating crystallization in moderate temperatures. The higher salinity has impact to speed up the dissolution process of cuprous oxide (Cu<sub>2</sub>O), a common binder in soluble antifouling paints where the performance of antifouling paints is more efficient in seawater compared to that in estuary water.

# **3. 2. Visual Examination of Exposed Specimens** The usage of anticorrosion and antifouling paints A and B as primary specimens in preceding research [19] is also utilized in the present research. All of the paints A and B specimens after being exposed to seawater are shown in images in Tables 2, 3, 4, and 5. The use of both AFP-A and AFP-B, compared to both AC paint A and AC paint B, could reduce the growth and settlement of marine biofouling organisms for up to 12 months.

Table 6 shows biofouling percentage on antifouling paint surface after certain field exposure. On the basis of results, the percentage of adherent biofouling increased gradually with the exposure time up to 12 months for both antifouling paints. The attachment of biofouling occurs at 6 months of exposure. The percentage of biofouling type A antifouling paint is less than type B antifouling paint.



Depth of the sea (m)	AC paint A	AF paint A	Depth of the sea (m)	AC paint B	AF Paint B
0	S COL	• • • • • • • • • • • • • • • • • • •	0	5.00	5 cm
1		20 0 5 cm	1	<u>5 em</u>	7922 - Mb
2	5 cm	4 13 cm	2	3 on	5 cm
3			3	÷ cm	<u>5 cm</u>

TABLE 3. Visual observation of samples after three months of exposure

TABLE 4. After six months of exposure, the visual examination of representative specimens



In the present research, tubeworms and barnacles are apparently some of the most significant and visible marine biofouling organisms on both AC paints during exposure. Mature barnacle species started appearing on both AC paints in 6 months of exposure. There is no or less different of marine biofouling growth distribution on both type of AC paints in different depth of the sea and various exposure times. The homogeneity of biofouling distribution on the samples of AC paint is caused by the installment of field test racks in euphotic zone where seawater quality parameters were almost the same in that zone. Furthermore, the existence of barnacles and tube worms as most attached biofouling organisms are categorized as calcareous macrofouling (30). Moreover,

Depth of the sea (m)	AC paint A	AF paint A	Depth of the sea (m)	AC paint B	AF Paint B
0		.5 cm	0		5 cm
1		Sem	1		

TABLE 5. After twelve months of exposure, the visual examination of representative specimens

**TABLE 6.** Biofouling percentage on antifouling paint surface after certain field exposure

Depth of the sea (m) AC AF Paint A Paint (%) A (%)	Depth of the sea (m) 0	AC Paint B (%)	AF Paint B (%)				
	0	100					
0 100 0	1	100	0				
1 100 0	1	100	0				
2 100 0	2	100	0				
3 100 0	3	100	0				
3 months	of exposure						
Depth of the sea (m) AC AF Paint A Paint (%) A (%)	Depth of the sea (m)	AC Paint B (%)	AF Paint B (%)				
0 100 0	0	90	0				
1 90 0	1	90	0				
2 70 0	2	85	0				
3 100 0	3	100	0				
6 months of exposure							
Depth of the sea (m) AC AF Paint A Paint (%) A (%)	Depth of the sea (m)	AC Paint B (%)	AF Paint B (%)				
1 100 5	1	100	35				
2 100 5	2	100	10				
12 months of exposure							
Depth of the sea (m) AC AF Paint A Paint (%) A (%)	Depth of the sea (m)	AC Paint B (%)	AF Paint B (%)				
0 90 5	0	90	40				
1 90 5	1	80	35				

numerous different bacterial colonies are typically discovered on AC paints during the initial stages of biofouling growth, and these colonies serve as the principal nutrition for the growth of macroorganisms after few days to many weeks of exposure. Due to the ideal habitat of seawater, it can be assumed that marine biofouling will continue to grow and mature over month of exposure as well as the present results.

3.3. The Inhibitive Mechanism of Antifouling Paint against Marine Biofouling Figures 6 and 7 show cross sections of both AF paints, each of which has a three-layer coating consisting of a primer coating (the first layer), an intermediate coating (the second layer), and a top coating (AF layer). Before exposure, the average AF layer thickness of the two multiple systems of AFP-A and AFP-B was 226 µm and 116 µm, respectively. On the basis of the results, AF coating layer thickness decreased for both AFP-A and AFP-B during field exposure up to 12 months. In Figures 8 and 9, the AF coating layer thickness reduction on AFP-A is less than that on AFP-B after exposure. AF layer is not present in AFP-B after 12 months of exposure compared to AFP-A after 12 months of exposure. The difference in thickness loss of both AF paints after exposure is presumed due to the different initial thickness of AF coating layers. Moreover, the initial thickness of coating value prior to exposure is used to estimate the service life of AF paints (19, 31, 32) as well as recent study. It suggests that the initial thickness of the AF coating layer up to 12 months of field exposure determines the service life of the AF paint system.

In recent work, both of AFP-A and AFP-B is classified as tin-free-polishing copolymer (tin-free SPC) which based on silyl acrylate (SA) as primary binder according their technical data sheet. The efficacy of tin-free SPC AF paints is related to the ability of that paint which inhibit the growth and settlement of biofouling in controlled



Figure 6. Prior to exposure, a cross-section picture of Paint A



Figure 7. Prior to exposure, a cross-section picture of Paint B



**Figure 8.** Cross-sectional pictures of Paint A that are representative after (a) 3 months of exposure, and (b) 12 months of exposure to seawater at a depth of 1 m

release rate of binder matrix. That ability could make to control the loss rate of AF paints thickness during field service compared to other type of AF paints such as hard AF paint and ablative paint. The inhibitive mechanism of SPC-AF paint against the settlement and growth of marine biofouling, the ingress of seawater takes place into the



**Figure 9.** Cross-sectional pictures of Paint B that are representative after (a) 3 months of exposure, and (b) 12 months of exposure to seawater at a depth of 1 m

paint matrix, dissolve gradually all additives such as primary biocide, co-biocides and others to environment. That process takes place simultaneously and repeatedly which create a thin leached layer of AF coating without main dissolved additives such as Cu<sub>2</sub>O and ZnO. The absence of soluble primary biocide, such as Cu<sub>2</sub>O, results in pores being left in the matrix paint, which can be defined as a leached layer.

Furthermore, the leaching process of SPC AF paint comprises two sections such as initial leaching and steadystate leaching. When a freshly painted surface comes into touch with seawater environment and a biocide additive begins to dissolve at the top layer of AF paint, the leaching process for the painted structure begins immediately. The main ingredients used to formulate AF paints: solvent, binder, biocide, booster biocide, extenders, pigments, and miscellaneous additives (19). Generic Cu<sub>2</sub>O is used as the primary inorganic biocide in both types of AF paints A and B, with co-biocides like ZnO additive also added to enhance the suppression of micro- and macro-algae growth and settlement. The presence of CuPt compound is necessary to boost the performance of primary biocide. Moreover, the following chemical Equation 1 is the proposed mechanism of the primary biocide of Cu<sub>2</sub>O dissolving in seawater:

$$Cu_{2}O(s) + 2H^{+}(aq) + 4Cl(aq) \rightarrow 2CuCl^{-}(aq) + H_{2}O$$
(1)

The presence of a high concentration of chloride ions, which increases the rate at which  $Cu_2O$  dissolves, is

correlated with salinity levels of a high magnitude. In initial stage, when Cu<sub>2</sub>O additive firstly contacts with sea water, that process yields soluble hydrated Cu(I) chloride complexes. That complexes compound is rapidly oxidized to  $Cu^{2+}$  ion as the main biocidal species against biofouling. The mechanisms of controlled release rate of biocides and co-biocides such as diffusion and chemical reactions where binder reaction, seawater water soluble pigments dissolution and polishing processes take place concurrently. In addition, those mechanisms could govern the magnitude of thin leached layer thickness for SPC AF paint. It is presumed that the disappearance of mostly biocide and co-biocide additives in silyl acrylate matrix creates many small pores in that matrix and enhances the magnitude of total wetted area on top surface of AF paint. During operational service, the wettability of the binder changes from hydrophobic to hydrophilic, causing the hydrolysis reaction to occur through the layer of AF coating that has been leached. Because partially reacted binder tends to be eroded by the motion of seawater and exposed at a less reacted AF layer surface, the AF coating has a self-polishing action. Biocides and co-biocides enriched matrix are present in the less-reacted AF coated surface or no leached layer zone, which inhibits the growth of marine biofouling. After completing the initial stage of leaching process, the steady-state leaching process starts simultaneously. In steady-state conditions, the rate of AF binder erosion caused by mechanical activity such as saltwater tide, current, and vessel movement is equal to the diffusion of ions from seawater bulk through the leached AF layer. The rate of biocide release from paint matrix is affected by seawater current, where leached AF layer can be eroded of polished easily. The role of seawater current rate is essential for the reduction of AF coating layer during service. The crucial function of the tidal current is its ability to easily wear or erode a leached layer of the AF layer, producing a fresh surface of the biocide-enriched layer. The simultaneous AF layer leaching process continues until there is no AF layer present during service. Therefore. It is pressumed that the thickness factor of SPC-AF paint can increase its lifespan during operational services at coastal aquifers of North Jakarta

# 4. CONCLUSIONS

The performance of both self-polishing copolymer (SPC) antifouling paints A and B showed remarkable efficacy compared to anticorrosion paints A and B in North Sea of Jakarta, Indonesia against the settlement of marine biofouling especially tubeworm and barnacle species. During operational service, the physical and mechanical properties of the AF paints are not significantly affected by variations in sea level up to 3 meters of depth and certain period of exposure such as pencil hardness, gloss

and adhesion strength. In both AF paints A and B, the presence of a primary biocide like  $Cu_2O$  may minimize the growth and establishment of marine biofouling at coastal aquifers of North Jakarta. The seawater parameter such as salinity, water temperature, sea current and pH has a greater impact on the gradual lossed thickness for AF paints due to the dissolution of  $Cu_2O$  and other additives to seawater. The dissolution of  $Cu_2O$  took place in both initial and steady-state leachings of SPC-AF paint during service.

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بیوساید مبتنی بر مس بیشتر به عنوان افزودنی اولیه رنگ ضد رسوب (AF) در اندونزی به ویژه در مخازن استفاده می شود. ارزیابی کارایی رنگ AF در جایی انجام شد که رنگ ضد خوردگی (AC) نیز به عنوان مرجع بود. پانل ها با هر دو رنگ تا دوازده ماه در معرض اعماق دریاهای مختلف تا سه متر قرار گرفتند. اندازه گیری پارامترهای آب دریا شامل هدایت آب، pH، دما، اکسیژن محلول و شوری انجام شد. بر روی پانل های رنگ آمیزی شده با AF، رسوب زیستی دریایی چسبیده یا کمتری وجود نداشت، اما در پانل های رنگ شده با AC تا دوازده ماه قرار گرفتن در معرض میدان در اعماق مختلف دریا وجود نداشت. هیچ تفاوتی بین خواص رنگ های AF قبل و بعد از قرار گرفتن در اعماق مختلف دریا وجود نداشت. عملکرد بازدارنده رنگ AF به وجود لایه AF حاوی بیوسید Cu2O بستگی دارد که در آن ضخامت آن لایه با افزایش زمان قرار گرفتن در معرض كاهش مي يابد.

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### Laser Scanning Speed Influences on Assessment of Laser Remelted Commercially Pure Titanium Grade 2

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ABSTRACT

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Keywords: Commercially Pure Titanium Laser Re-melting Microhardness AFM Analysis Pitting Corrosion In this research, the influences of laser surface remelting using different scanning speeds on the microstructure, roughness, and hardness of Commercial pure Titanium (Grade 2) were investigated. High power Nd: YAG pulsed laser was used. The laser scanning speeds used in this study were 4, 6, 8, and 10 mm/s and the other laser parameters (power, pulse frequency, beam diameter) were constant. The corrosion performance of the laser surface remelted and Cp titanium was then evaluated by potential dynamic measurements in a 3.5% NaCl solution. The results revealed that due to the diffusionless transformation after laser surface treatment and the formation of the martensite phase, the surface post-laser treatment was significantly different from those before the treatment. The results were indicated using an optical microscope, FE-SEM, XRD, AFM, and microhardness angles are grain size (26.06 nm) due to the high input energy and slow cooling rate, while the highest scanning speed (10 mm/s) had the greatest microhardness (291.5 Hv) due to the short interaction time between the substrate surface and laser beam and the higher cooling rate. The results also demonstrated the obvious improvement in the pitting resistance of Cp Ti in harsh environments as a result of the influence of laser remelting.

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#### **1. INTRODUCTION**

In recent years, titanium as a metal and its alloys have attracted interest as a material in the marine, spacecraft, automotive, petrochemical, biomedical, and energy industries as well as steam condensers in the power generation industry (1, 2). Titanium alloy has great properties due to its high strength-to-weight ratio, low

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density, and high corrosion resistance (3, 4). Despite these excellent properties and high affinity for oxygen reaction to form spontaneous beneficial surface oxide film. However, any breakdown of the passivity film can lead to a localized attack such as pitting corrosion (5, 6). Furthermore, the absence of an oxygen source condition may result in the disability of regenerating this protective film (7). Surface engineering is a field of science that includes design, modification, and technique to enhance the performance of the bulk surface for different chemical, physical, and mechanical properties (8, 9). Surface engineering is crucial to providing high-quality services and preventing failure for an extended time (10). Surface modification of Cp Ti is considered an effective method to improve pitting corrosion (11). Modifying the microstructure of the base metal plays an important role in the improvement of performance (9). Laser surface remelting (LSR) is an emerging processing technology that involves rapid melting and cooling when a laser beam passes through a small localized region on a sample surface (12). LSR can remarkably provide metastable crystalline phase and grain refinement on the Ti alloy surface without compromising its bulk mechanical properties (13). The best results can be obtained from the laser beam interacting with the surface by controlling the process-independent parameters such as power, speed, pulse energy, etc. This enables highly accurate control of the depth, extension, and temperature change of the region subjected to the radiation of a laser, which may also be observed. Due to its outstanding adaptability and chemically clean processing methods, materials surface processing procedures can be provided with high added value and with respect for the environment. Laser treatment of materials produces no chemicals or significant waste. These characteristics lead to high processing speeds and inexpensive costs, which have an impact on applications involving the processing of materials (14). The primary laser parameters that can be influenced during processing are laser power, beam radius, specimen or work-piece velocity, and beam mode, which can be stationary, rotating, top hat, or Gaussian. In addition, the alloy's composition and concentration, as well as the concentration and flow rate of any processingrelated gases, like nitrogen in the case of alloying. Further important factors include the dimensions, particularly the workpiece's thickness and its capacity to absorb laser energy (14). Furthermore, with increasing scanning speed, the remelting depth decreased (15). As the laser power rises, the roughness parameters increase too (16). There are few attempts in the literature to explain the detailed information of titanium alloys using laser treatment. Sun et al. (15) investigated the influence of laser remelting on the corrosion behavior of Cp Ti (Grade 2) in 3% NaCl. It was discovered that laser surface remelting significantly increased pitting potential. Bahloul et al. (16) used a short pulse Nd: YAG laser treatment to increase the surface corrosion resistance and fretting wear of Ti plates (Grade 4) by raising the surface hardness. The objective of this paper is to study the influence of laser remelting scanning speed on the general surface properties assessment of Cp Ti (Grade 2). However, the microstructure, phase, morphology, microhardness, and corrosion resistance have been reported. We leveraged the versatile cooling rate capabilities of laser surface remelting to vary critical microstructure attributes within the melted zone. This is done by altering the laser scanning speed of the Laser surface remelting.

#### 2. MATERIALS AND METHODS

**2. 1. Materials Characterization** A square-shaped commercially pure titanium Cp Ti (grade 2) specimen of dimensions 15 mm\*15 mm\* 3 mm was chosen as the substrate material. Table 1 shows the chemical composition of the Cp Ti substrate as received from the supplier was agreed with ASTM B265 (17).

2. 2. Laser Treatment A PMT4297 model (Nd: YAG) pulsed laser has been utilized as the laser surface treatment (LST) platform. It emits radiation on a single wavelength of 1064 nm. The laser beam was focused on the specimen surface placed with suitable clamped onto a CNC table and scanned over the surface of specimens to generate a controlled overlap. The laser was operated with a typical repetition rate of 2 Hz. The overlapped tracks of approximately 25% were carried out to cover all the surface of the specimens. To select the best laser parameters for overlapping, it's essential to make a careful analysis of laser processing parameters. As indicated in Table 2, several experiments were conducted with various scanning speeds and constant values for other parameters (power, pulse frequency, and beam diameter). The shrouding gas for the laser-generated melt pool was argon gas.

**2. 3. Characterization Techniques** Various analytical techniques were used for the characterization of the Cp titanium before and after laser treatment. The

**TABLE 1.** Chemical composition of CP Ti grade according to ASTM B 265

C, max.	Element	H, max.	N, max.	O <sub>2</sub> max.	Fe max.	Other Elements max. each	Other Elements, max. total
0.08	Standard	0.015	0.03	0.18	0.2	0.1	0.4

surface microstructure was monitored by optical and Field emission scanning electron microscope (FESEM). X-ray diffraction test (XRD) was used to present the phases of Cp Ti before and after laser treatment. Topography, nano roughness, and grain size were determined using an Atomic Force Microscope (AFM). Vickers microhardness (Hv) measurements were evaluated using a (TH714) tester under 300g load for 15s. The corrosion rate in (mm/y) was determined using the polarization method after immersion in 3.5% NaCl by using a CHI 604e electrochemical system.

#### **3. RESULTS**

3. 1. Microstructure Results To study the effect of laser parameters on the general properties of Cp Ti, it's important to the microstructure's alterations from a top surface. As illustrated in Figure 1 (a, b), optical and FESEM images revealed that the Cp Ti is composed of a single alpha ( $\alpha$ ) phase that has been transformed to an acicular martensite phase  $(\alpha')$  as a result of the high cooling rate and diffusionless transition. Figure 1(a) shows that the  $\alpha$  phase grains are intermingled with small yet noticeable pockets of beta ( $\beta$ ) grains, these beta pockets formed as a result of the presence of minor impurities (O<sub>2</sub>, H, N, C, Fe) that revealed in Table 1. About 98 % or more alpha phase ( $\alpha$ ), the remaining being iron stabilized beta phase (18). While Figure 2 reveals the plate-like microstructure of martensite  $(\alpha)$  that has a hexagonally packed crystal structure (HCP). As the laser intensity is highest in the middle of the pulses and decreases as one moves toward the sides of the pulse, the alpha prime martensite plates ( $\alpha$ ') were oriented toward the heat transfer direction (16). This is the reason for the beach marks on the edges of the pulse revealed in Figure 1(b).

Figure 3 displays the optical microscope images of the laser tracks on the (Cp Ti G2) substrate at various scan speeds. On the surface of Cp Ti, it can be noticed

**TABLE 2.** The laser processing parameters used in laser surface treatment of  $C_P$  Ti in this investigation

Laser parameters	Track No.1	Track No.2	Track No.3	Track No.4
Power (W)	800	800	800	800
Pulse frequency (Hz)	2	2	2	2
Traverse speed (mm/s)	10	8	6	4
Interaction time (s)	0.08	0.1	0.133	0.2
Beam diameter (mm)	0.8	0.8	0.8	0.8
Heat input (J/mm)	80	100	133.33	200



**Figure 1.** Optical micrographs showing the key microconstituents for the Cp Ti substrate (a) As it is at magnification 125x (b) After laser treatment at magnification 10x



**Figure 2.** FESEM image of Cp Ti after laser treatment showing the plates-like structure of martensite phase  $(\alpha)$ 

that as the laser speed decreased, the number of pulses per unit area increased (1.4 for the 10mm/s speed and 1.5 for the 4mm/s speed). Lower laser scanning speeds give the laser beam more time to alter the surface and more opportunities to produce more pulses on the Cp Ti surface (19).

The relationship between the number of laser pulses per unit area and laser speed is revealed in Figure 4. With increasing the laser speeds (4,6,8,10 mm/s) the heat input was deceased (200, 133.33, 100, 80J/mm, respectively) because as speed increased the interaction time decreased between the laser and substrate.



(d)

**Figure 3.** Shows the effect of laser scanning speed on the number of pulses per unit area. (a) Track No.1at V=10mm/s (b) Track No.2 at V=8mm/s (c) Track No.3 at V=6mm/s (d) Track No.4 at V=4mm/s

**3. 2. AFM Results** The topography and roughness of the Cp Ti surface were observed using AFM as shown in Table 3, and Figure 5. The results show that as the laser scanning speed increased, the surface roughness increased. Since the size of grains depends on the rate of



Figure 4. Shows the relationship between No. of laser pulses per unit area and laser speed

**TABLE 3.** surface topography and roughness for the laser tracks analyzed by AFM

	J J			
No. of Track	Laser Speed (mm/s)	Sa (nm)	Sq (nm)	Grain dia. (nm)
1	10	6.180	8.948	61.05
2	8	5.454	7.849	57.93
3	6	1.637	2.208	39.39
4	4	1.177	1.499	26.06

cooling, the higher the cooling rate and higher thermal gradient (at the lowest laser speed of 4 mm/s) the smaller the size of grains (26.06nm) which agrees with reported data by Mahamood et al. (20). The relation between roughness and laser scanning speed can be revealed in Figure 6. It's important to note the AFM roughness values were taken from the middle of the pulse. The track with a laser speed of 4mm/s had minimal roughness (1.499nm), while the track with the highest laser scanning speed of 10mm/s in the investigated study had a higher roughness (8.948nm). Because the pulse edges were rougher than the middle due to the gradient of heat distribution. The track at 6 mm/s has a lower range of grain diameter (homogenous distribution) along the surface Figure 5g after laser remelting if compared with the rest tracks. The effect of heat input on the resultant grain diameter of different laser scanning speeds on Cp Ti can be clearly observed in Figure 7.

**3.3.XRD Results** Phase identification of the Cp Ti before and after the laser surface treatment was established from an X-ray diffraction pattern. As illustrated in Figure 8 the Cp Ti before laser treatment had alpha ( $\alpha$ ) microstructure Figure 8a and it would transform to martensite structure ( $\alpha$ ') Figure 8b after the surface laser treatment due to the diffusion-less transformation and high cooling rate (15).

After laser remelting to the surface, the peaks become sharper as a result of the crystallinity.





**Figure 5.** AFM 3D height surface topography of laser tracks on Cp Ti G2 at (a) 10 mm/s scanning speed (b) 8 mm/s scanning speed (C) 6 mm/s scanning speed (d) 4 mm/s scanning speed (e), (f), (g), (h) reveals the grains agglomeration at 10 mm/s, 8 mm/s, 6 mm/s, and 4 mm/s respectively



Figure 6. Shows the relationship between roughness and laser scanning speed



**Figure 7.** Shows the variation of heat input and grain diameter resulting from AFM analysis with laser scanning speed used in this investigation



**Figure 8.** XRD of (a) Cp Ti and (b) after surface laser treatment shows the phase transformation from alpha to the martensite phase

**3. 4. Microhardness Results** Vickers microhardness was also used to evaluate the tracks after laser remelting of Cp Ti at various laser scanning speeds. As the laser scanning speed increased the hardness

increased as shown in Table 4. The laser-material interaction time is low at higher laser scanning speeds, and subsequently higher cooling rate and thermal gradient than the lower laser scanning speeds. Rapid solidification and cooling that occurred at high laser speed induced a higher microhardness value which agrees with reported data by Tavakoli et al. (21).

The effect of heat input and interaction time between the laser beam and Cp Ti can be observed in Figure 9. This reveals the gradients of microhardness values depending on heat input in the region of laser – CpTi interaction. The maximum microhardness can result from higher scanning speed and lower heat input. That means the heat transfer was higher than at high heat input and subsequently higher cooling rate.

In order to determine the corrosion rate of the Cp Ti after laser treatment, it must overlap the tracks on the surface. So, it's necessary to select the best suitable parameters of the laser remelting process to overlap. Track No. 3 with a scanning speed of 6 mm/s was selected to produce the overlapped samples. Due to the results obtained from tests previously as illustrated in this study. The appearance of the surface after laser treatment is shown in Figure 10, which also exhibits successful laser overlap over the whole Cp Ti surface. It can observe the distribution of pulses throughout the surface.

**3. 5. Chemical Corrosion Results** Despite of excellent corrosion resistance of Ti, further improvement

**TABLE 4.** Revealed the microhardness results at each laser scanning speed using Vickers microhardness analysis

No. of Track	Laser Speed (mm/s)	Microhardness Value (Hv)
1	10	291.5
2	8	251
3	6	220.9
4	4	219.3



Figure 9. Indicates the relationship between microhardness, interaction time of the laser beam, and heat input of the different laser scanning speeds used in this investigated study



Figure 10. Surface appearance after the pulsed laser surface remelting at 6 mm/s scanning speed

is still required. In order to enlarge Ti application areas in severe environments. Laser surface remelting of Ti could be a promising tool to be approved in this area. The corrosion rate in millimeters per year (mm/y) for the asreceived Cp Ti substrate and the substrate after laser treatment was evaluated by using an electrochemical system. The OCP value was increased from - 0.383 to -0.362 volts after surface laser treatment of the Ti substrate. This pushed the corr. potential upward, indicating that the laser treatment increases substrate surface protection, as shown in Figure 11. Also, it can be observed from the curve after laser remelting, that the voltage decreases but returns and rises by virtue of the laser treatment that changes the properties of the surface layer that is subjected to interaction with the solution. When comparing the curve with the condition before laser treatment, it was found that the voltage decreases gradually and continuously.

Tafel plots in Figure 12 revealed that there are no pitting corrosion sites before and after the laser treatment (negative loop) during immersion of the laser-treated substrate in the salt solution. However, despite that, the laser treatment showed an additional improvement through the decrease in the value of the current density from  $7.969*10^{-7}$  to  $3.969*10^{-7}$  Amp which agree with



Figure 11. OCP curves for the Cp Ti before and after the laser treatment



**Figure 12.** Cyclic polarization behavior for the base Cp Ti substrate and the Cp Ti substrate after laser treatment in 3.5% NaCl solution

reported data by Tavakoli et al. (21). Furthermore, there is a noble shift of the curve if compared with untreated Ti. The E. corr decreased (from -0.194 to -0.223 volt) after the protection of the Ti surface using laser treatment. Due to the martensitic phase transformation and rapid solidification resulting from laser surface remelting which lead to decreased corrosion rate (15). Table 5 gives the potentiodynamic corrosion results of samples before and after the surface treatment. These findings indicated that the probability of pitting prediction and propagation is very low.

**TABLE 5.** Chemical corrosion parameters and results

ITEM	E corr. (volt)	I corr. (Amp.)	Corr. Rate mm/y	OCP (volt)
Ti substrate	-0.194	$7.969\times10^{7}$	$1.806 \times 10^{-2}$	-0.383
Laser on Ti substrate	-0.223	$3.969\times10^{-7}$	8.995×10 <sup>-3</sup>	-0.362

#### 4. CONCLUSION

The variation of microstructure, morphology, constituent phases, microhardness, and corrosion resistance of a laser-remelted Cp Ti with changing laser scanning speeds have been studied. The laser scanning speed was varied between 4 and 10 mm/s. The results revealed the obtaining of a completely different microstructure as a result of rapid cooling rates. As the scanning speed decreases, the surface roughness and average grain diameter decrease. Microhardness values increased with increasing the laser scanning speed. The maximum value of microhardness in this investigated study was 291.5 Hv. at a scanning speed of 10 mm/s. Due to the short interaction time between the substrate surface and laser beam and high cooling rate. Also, this study demonstrated the obvious improvement in corrosion resistance after laser remelting of the Ti surface. Laser surface remelting leads to a decrease in the corrosion rate from  $1.806 \times 10^{-2}$  to  $8.995 \times 10^{-3}$  mm/y and enlarges the materials application range in severe service environments.

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#### Persian Abstract

#### چکیدہ

تأثیر ذوب مجدد سطح لیزر با استفاده از سرعتهای مختلف روبشی بر روی ریزساختار، زبری و سختی تیتانیوم خالص تجاری (درجه 2) در این تحقیق مورد بررسی قرار گرفت. از لیزر پالسی Nd:YAG با توان بالا استفاده شد. سرعت اسکن لیزر مورد استفاده در این مطالعه 4، 6، 8 و 10 میلیمتر بر ثانیه و سایر پارامترهای لیزر (قدرت، فرکانس پالس، قطر پرتو) ثابت بودند. عملکرد خوردگی سطح لیزر دوباره ذوب شد و CP تیتانیوم سپس با اندازه گیریهای دینامیکی بالقوه در محلول %NcI 3.5% ارز از قدرت، فرکانس نشان داد که به دلیل تبدیل بدون انتشار پس از درمان سطحی لیزر و تشکیل فاز مارتنزیت، تیمار پس از لیزر سطح به طور قابل توجهی با قبل از درمان متفاوت بود. نتایج با استفاده از میکروسکوپ نوری، AFM FE-SEM، محلح لیزر و تشکیل فاز مارتنزیت، تیمار پس از لیزر سطح به طور قابل توجهی با قبل از درمان متفاوت بود. نتایج با انرژی ورودی بالا و سرعت خنک کنندگی پایین، کمترین زبری و کمترین اندازه متوسط دانه (20.60 نانومتر) را دارد، در حالی که بالاترین سرعت اسکن، 4 میلیمتر بر ثانیه، به دلیل انرژی ورودی بالا و سرعت خنک کنندگی پایین، کمترین زبری و کمترین اندازه متوسط دانه (20.60 نانومتر) را دارد، در حالی که بالاترین سرعت اسکن، 10 میلیمتر بر ثانیه، به دلیل است. بیشترین ریزسختی (یراست در 20.50) را به دلیل زمان اندرکنش کوتاه بین سطح بستر و پرتو لیزر و سرعت خنک کنندگی بالاتر داشت. نتایج همچنین بهبود آشکار مقاومت حفرهای CPT را در محیطهای سخت در نتیجه تأثیر ذوب مجدد لیزر نشان داده.



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### Energy Efficiency with Internet of Things Based Fuzzy Inference System for Room Temperature and Humidity Regulation

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### ABSTRACT

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Energy consumption is a crucial aspect in the effort to optimize the utilization of resources and reduce energy wastage. Focusing on energy efficiency can result in operational cost savings, a reduction in greenhouse gas emissions, and support for environmental sustainability for future generations. Therefore, it is important to consider energy efficiency in daily life, especially in the use of electricity for electronic devices. This research aims to compare the energy efficiency of two different approaches to Air Conditioner (AC) usage: the manual method and the fuzzy logic method. The manual method involves eight tests with direct power measurements over a 30-minute period at various AC temperature settings, namely 18°C, 20°C, 23°C, 24°C, 25°C, 26°C, 27°C, and 30°C. On the other hand, the fuzzy logic method involves six tests allowing for dynamic temperature adjustments based on room conditions. The research findings indicate that the fuzzy logic method achieves lower average power consumption. except at 30°C, where the manual method is slightly more efficient (a difference of 140,745 watts). This difference is primarily attributed to the "cooling and fan" mode used at lower temperatures in the manual method, resulting in higher power consumption. Furthermore, this research reveals the potential of the fuzzy logic in optimizing AC power usage based on real-time conditions, achieving approximately a 41.96% energy savings. The primary contribution of this study is to provide practical insights into how the fuzzy logic method can significantly reduce AC energy consumption, support energy efficiency efforts, and contribute to environmental sustainability.

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#### **1. INTRODUCTION**

The Internet of Things (IoT) has become one of the most prominent technologies in the evolving digital era (1-5). IoT has transformed the way humans interact with devices and systems in their surroundings, ranging from smart homes to autonomous vehicles (6-8). IoT is often integrated with artificial intelligence (AI) (9). One area where IoT has made a significant contribution is in enhancing comfort and energy efficiency in the environment, especially in regulating room temperature and humidity (10-12). The regulation of room temperature and humidity is a crucial aspect of creating a comfortable and productive environment. Excessive heat or cold, as well as inappropriate humidity levels, can disrupt the comfort and health of room occupants. Moreover, inefficient regulation of temperature and humidity can lead to energy wastage, negatively impacting the environment, both directly and indirectly.

Currently, tools widely available in the market tend to favor manual settings, such as the implementation of the ON/OFF system. This manual method is inefficient in energy usage because it is unresponsive to minor temperature fluctuations, does not consider humidity, and results in significant energy wastage. The consequences include increased energy costs, excessive utilization of natural resources, inconvenience to room occupants, and an overall decrease in energy efficiency.

In an effort to effectively enhance the regulation of room temperature and humidity, Fuzzy Inference Systems (FIS) have emerged as efficient solutions (13-15). FIS is a regulatory method rooted in fuzzy logic, enabling machines to make decisions based on multiple influencing variables (16). In the context of regulating

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room temperature and humidity, FIS empowers IoT devices to intelligently manage indoor temperature and humidity based on specified parameters. Therefore, in this study, researchers will investigate energy consumption when employing FIS and IoT to control room temperature and humidity using AC. Energy consumption plays a pivotal role in achieving resource efficiency (17-19).

This research aims to reduce unnecessary energy consumption, safeguard the environment, promote sustainability, enhance productivity, foster technological innovation, and improve quality of life. By developing more efficient solutions, this research yields benefits in the form of energy conservation, reduction in greenhouse gas emissions, enhanced operational efficiency, adoption of intelligent technologies, and the creation of a more comfortable and healthier environment. This objective directs the transition towards wiser, more sustainable, and more impactful energy utilization for individuals. This research represents a continuation of prior studies on temperature and humidity control systems utilizing FIS and IoT-based AC (20). However, this study specifically concentrates on devising an effective and efficient AC control system for regulating room temperature and humidity using Tsukamoto's FIS and IoT methods, without evaluating the efficiency of energy consumption, both in the short-term and long-term usage (20). Particularly, it addresses the utilization of long-term AC systems, which are categorized as inefficient (21-23).

Previously, Orhan Ekren and Serhan Küçüka had conducted research on fuzzy logic-based control algorithms for regulating compressor speed and Electronic Expansion Valve (EEV) opening percentages in chiller systems. This research aimed to enhance the efficiency of the chiller system by utilizing a Variable Speed Scroll Compressor (VSSC) and EEV. Fuzzy logic algorithms were employed to govern the compressor speed based on the chiller water output temperature, while the opening percentage of the EEV was controlled based on the refrigerant superheat value at the evaporator outlet. The study's findings revealed a performance improvement of 17% when compared to thermostatically controlled fixed-speed chiller systems, as well as superior control over water temperature achieved through the use of fuzzy-controlled VSSC (24).

Ahmed et al. (25) proposed a scheme utilizing fuzzy logic to control central air conditioning and maintain room temperature and humidity close to predefined targets. This aims to reduce electrical energy consumption and create comfort in various rooms of different sizes and conditions. The result is comfortable rooms with higher energy efficiency. Subsequently, Riyadh Waheed et al. (26) highlighted the role of fuzzy logic-based controllers in enhancing the efficiency of air conditioning, especially in classrooms. The research findings indicated that fuzzy logic-based controllers are superior in regulating room temperature and humidity compared to traditional controllers.

By the use of fuzzy logic controllers in air conditioning systems Francis et al. (27) have successfully reduced electricity consumption by adjusting the compressor speed and operating mode according to environmental conditions and user needs. This demonstrates significant potential for energy savings in air conditioning systems, particularly in urban areas, while considering various input parameters such as temperature, occupancy, time, and weather conditions. A review by Belman-Flores et al. (28) stated that the use of fuzzy logic controllers in refrigeration and air conditioning systems (RACs) has proven their ability to improve thermal efficiency compared to classical controllers like ON/OFF and PID. Computer simulations and experimental tests also showed that the use of fuzzy controllers can reduce energy consumption.

In another study, Nasution (29) evaluated vehicle AC systems using Fuzzy Logic Control (FLC) algorithms to continuously regulate compressor speed. Experiments were conducted with variations in set point temperature, internal heat load, and compressor speed. The results demonstrated that the utilization of FLC led to significant energy savings and improved indoor comfort when compared to conventional ON/OFF controls. This technique holds the potential to enhance the efficiency and overall performance of passenger vehicle AC systems. Furthermore, this research is corroborated by a study conducted by Khayyam et al. (30) who also discussed the development of intelligent energy management systems for optimizing the utilization of AC systems in vehicles. The system incorporates data from various information systems to make intelligent decisions, including predicting road power demand and employing intelligent control strategies. Simulations indicate that this system can achieve energy savings of up to 12% when compared to conventional systems and other energy management systems.

Additionally, the efficacy of Fuzzy logic in attaining energy efficiency is further supported by other studies, such as those conducted by Chu et al. (31). This study proposed the use of the Least Enthalpy Estimator (LEE) in the Fan Coil Unit (FCU) controller in Heating, Ventilating, and Air Conditioning (HVAC) systems to conserve energy and maintain thermal comfort levels. The LEE-based fuzzy FCU controller demonstrates the ability to accurately predict loads and adjust the FCU system's output based on temperature and relative humidity. Through experimentation, this controller successfully achieved the thermal comfort, energy efficiency, and reliability necessary in FCU control systems.

Regarding the efficiency of fuzzy logic, Saini et al. (32) also provided statements in their research supporting the efficiency achieved by fuzzy logic. Their study

utilized fuzzy logic to control loads in a Solar Home System with the aim of efficiently managing energy usage. Test results indicated that the use of fuzzy logic could reduce power consumption for lighting and fans compared to control without fuzzy logic.

While previous research has attempted to apply FIS and IoT in various contexts, such as solar home systems, chiller systems, or vehicle air conditioning, there is still a gap in research that focuses on room temperature and humidity regulation using AC with a comprehensive assessment of energy consumption. Previous studies often did not compare energy consumption between manual systems and fuzzy-based systems to understand the potential energy savings that can be achieved.

Therefore, in this study, we specifically examine room temperature and humidity regulation using AC while evaluating energy consumption. This research makes a stronger contribution to developing more efficient solutions for sustainable environmental control through AC usage by attempting to compare energy consumption between manual and fuzzy-based systems to determine potential energy savings.

#### 2. METHOD

The subsections outlined in this method section encompass three main aspects: the research stages, the application of fuzzy Tsukamoto, the specifications of the AC system used, and the methods employed for energy consumption analysis.

**2. 1. Research Stages** This research builds upon prior studies that primarily focused on assessing the environmental impact of AC systems following the implementation of fuzzy logic. The research process encompassed several stages, including requirements analysis, tool and application design, tool and application development, fuzzy logic integration into the tools, and testing the tools' impact on room conditions. These stages were systematically evaluated to attain the research objectives.

The developed tools and applications were then utilized to collect energy consumption data within AC systems. Subsequently, this data underwent analysis to gain insights into the influence of fuzzy logic on energy efficiency and the potential savings it can offer. As a result, this study aims to provide comprehensive and detailed insights into the impact of fuzzy logic on energy efficiency within AC systems. An overview of the research stages is illustrated in Figure 1.

**2. 2. Fuzzy Tsukamoto** The Fuzzy Tsukamoto model is a fuzzy logic-based control approach developed in past decades (33, 34). This approach combines the principles of fuzzy logic with intuitively defined



**Figure 1.** The research comprises two sets of stages: (a) stages that were previously conducted [20], and (b) the more advanced stages implemented in this study

linguistic rules to control complex and ambiguous systems. Fuzzy Tsukamoto utilizes the concept of fuzzy membership to depict uncertainty in system inputs and outputs. This concept allows system variables to exhibit varying levels of membership in different categories. For instance, in room temperature control, variables like "cold" and "hot" can have membership levels or fuzzy sets such as "slightly cold", "medium cold", "slightly hot", and "medium hot" (35). These membership levels describe the degree to which an input or output value belongs to a particular category. Linguistic rules are employed in the Fuzzy Tsukamoto model to establish connections between system inputs and outputs. These rules comprise conditional statements that link input conditions with output actions. For instance, "IF the room temperature is low, THEN the heating rate is increased". These rules are formulated based on expert knowledge in the relevant domain and are represented in the form of fuzzy sets.

Essentially, Fuzzy Tsukamoto is one of three models within FIS. The other two models are Mamdani and Sugeno reported in literature (36-38). FIS serves as a mathematical framework or model employed for implementing fuzzy logic in decision-making or system control (39, 40). FIS encompasses several key components that collaborate to generate outputs based on fuzzy inputs. FIS can find applications in various domains involving decision-making, system control, and the processing of uncertain or ambiguous data. Within FIS, existing human knowledge or expertise is represented in the form of fuzzy rules and applied to generate outputs based on given input conditions. FIS enables systems to process fuzzy data by amalgamating human knowledge with mathematical techniques, leading to more adaptable and flexible decision-making.

The control process utilizing Fuzzy Tsukamoto comprises several stages. Initially, the system input is transformed into fuzzy sets using membership functions. This initial stage is referred to as the fuzzification stage (41-43). Subsequently, linguistic rules are employed to establish connections between the fuzzy sets of inputs and the desired output. The subsequent stage involves the inference process, during which linguistic rules are assessed to generate the appropriate level of output membership. Lastly, the results of the inference are converted into crisp values through defuzzification, thereby producing numerical output that can be utilized for system control.

2.2.1. Fuzzification Fuzzification is the process of converting crisp (non-fuzzy) variables into fuzzy variables by using membership functions (20, 44, 45). Fuzzification allows mathematical representation of uncertainties in the system using fuzzy sets (44-48). The crisp variables that will be used as system inputs are converted into fuzzy sets using the membership function. The membership function associates the crisp value with the membership level in the fuzzy set. Each fuzzy set consists of a set of possible values for the relevant crisp variable. The membership function in fuzzification describes the extent to which a crisp value belongs to a fuzzy set. Membership functions are usually represented in the form of curves, such as triangular curves (49), trapezoidal curves, or other curves corresponding to the characteristics of variables and their domains. This curve shows the membership levels of variables in a fuzzy set at various points of their value.

Fuzzification is an important step in the fuzzy logicbased control process, as it converts crisp data into fuzzy representations that fuzzy systems can use to make decisions and produce appropriate outputs (50, 51). In combination with fuzzy inference and defuzzification, fuzzification assists fuzzy systems in modeling and controlling complex systems by taking into account the uncertainty and ambiguity inherent in system inputs. The fuzzification process is written in Equation 1.

$$x = fuzzifier(x_0) \tag{1}$$

where  $x_0$  is a firm value vector of an input variable, x is a fuzzy set vector defined as a variable, and fuzzifier is a fuzzification operator that converts a firm value to a fuzzy set (52).

2.2.2. Machine Inference At the inference system stage, fuzzy rules are used to draw conclusions based on fuzzy set theory and fuzzy rules in the form of IF-THEN statements (53). This IF-THEN statement can usually also consist of one or more antecedents (also called premises) located within the IF section with one or more consequent (also called conclusions) located within the THEN section. In general, a rule can have multiple premises associated with an AND statement (conjunction), an OR statement (disjunction), or a combination of the two. In this case, Zadeh identified three basic operators used in fuzzy rules, namely the AND, OR, and NOT operators (54, 55). The AND operator is used to retrieve the minimum element between the two fuzzy sets involved (56). In this context, the AND operator results in the lowest membership level of the corresponding fuzzy set (Equation 2). The OR operator, on the other hand, is used to find the maximum

element between two fuzzy sets. Using the OR operator, the highest membership level of the associated fuzzy set is taken (Equation 3). The NOT operator is used to subtract the value of 1 with a negated fuzzy element. In other words, if a fuzzy set has a membership level of  $\alpha$ , then using the NOT operator, the membership level becomes  $1 - \alpha$  (Equation 4) (57). In the context of this study, the AND operator is applied to each formed fuzzy rule. The use of this AND operator results in the lowest membership value of the fuzzy set involved in each of those rules. Mathematically, the AND operator can be described using Equation 2.

$$\mu K \cap L = \min(\mu K[x], \mu L[x]) \tag{2}$$

$$\mu KUL = \max(\mu K[x], \mu L[x])$$
(3)

$$\mu \mathbf{K}' = 1 - \mu \mathbf{K}(\mathbf{x}) \tag{4}$$

2. 2. 3. Defuzzification Defuzzification is a transformation that restates the output from a fuzzy domain into a crisp domain. Fuzzy output is obtained through the execution of some fuzzy membership functions. There are several methods that can be used in the defuzzification process, namely (1) Weighted Average Method (58-60), a method that calculates the average value by assigning a certain weight or weight to each element in the data set aimed at reflecting the relative importance or contribution of each element to the final result, (2) Mean-Max Membership (61-63), a method that combines several overlapping membership rules by taking the maximum value of each set membership at a point, then calculate the average of those maximum values, (3) Centroid (Center of Gravity) Method (64, 65), a method that calculates the center point (centroid) of a membership set using the weighted principle based on membership level. The membership value of each point on the set is multiplied by the position of that point, then added and divided by the total membership value, (4) Height Method (Max-Membership *Principle*) (66, 67), a method that takes the maximum value of the membership level in a membership set as a representation of the membership value of the entire set, (5) Center of Sums (68-70), a method that calculates the center of input values by adding input points and dividing them by the total number of inputs, (6) First (or Last) of Maxima (66, 71, 72), a method that selects the first (or last) point at which the membership level reaches the maximum value of a membership set as a representation of the overall membership value of that set, and (7) Center of Largest Area (73, 74), a method that calculates the center of the area of a membership set by taking the midpoint at the interval with the largest set area. The defuzzification method used in this study is the Weighted Average written in Equation 5.

$$\chi^{*} = \frac{\sum_{i=1}^{n} \mu c(\bar{x}_{i}) \bar{x}_{i}}{\sum_{i=1}^{n} \mu c(\bar{x}_{i})}$$
(5)

where  $\sum_{i=1}^{n}$  represents an algebraic sum with respect to the membership function of *n* fuzzy sets. This method has the limitation that it can only be used on fuzzy sets with symmetric membership functions (75).

2.3. AC Specifications Used As explained in the introduction, this study focuses on the analysis of energy consumption on the use of AC as an air conditioner. AC performance will be analyzed and evaluated to understand the impact of its use on power consumption after fuzzy logic is enacted in regulating AC values. One important step in power consumption analysis is obtaining the associated AC specifications. To collect AC specifications, first of all, it is necessary to know the electrical power consumed by the air conditioner. This information can usually be found on the technical specifications of the AC or on the label attached to the AC unit itself. This electrical power is expressed in units of watt (W) and is an important indicator for understanding the extent to which AC consumes power while operating.

Another important specification to know is the AC efficiency factor (76-78). The efficiency factor describes the level of efficiency of an AC in producing cooling relative to the power consumed (76). The efficiency factor is usually expressed as a percentage and can affect power consumption significantly. Therefore, knowing the efficiency factor of AC allows for more accurate calculations in estimating AC power consumption at different temperatures.

Based on the Decree of the Minister of Defense of the Republic of Indonesia No. 782/VIII/2015, the power standard for AC is calculated based on Paarden Kracht (PK) where 1 PK is equivalent to 0.7355 kW (79). While the AC used is equivalent to  $\frac{1}{2}$  PK, so  $\frac{1}{2}$  PK x 0.7355 kW = 0.368 kW. Then, the magnitude of  $\frac{1}{2}$  PK is equal to  $\pm$ 5000 BTU/h (British Thermal Units per hour) (80, 81). In addition, based on the reference read (82), the calculation of energy consumption per year can be obtained by Equation 6.

$$AE = \frac{Q * t}{EER}$$
(6)

where AE stands for "Annual Energy" which refers to the total energy consumed or used by a system, device, or equipment in a one-year period. Q is the Capacity that represents the cooling capacity or cooling load of the air conditioner. This capacity is measured in units such as BTU/h, kilowatts (kW), or tons. Capacity describes the amount of heat that an AC can remove in a given period of time. While t (operating time) refers to the operating time of the air conditioner. This is the amount of time that AC is used or operating in units such as hours, minutes, or seconds. While Energy Efficiency Ratio (*EER*) is the

ratio between the cooling capacity of AC and its input power. To calculate EER, you need to know the cooling capacity and AC input power in appropriate units, such as BTU/h and watts or kW. EER can be calculated using Equation 7 (83).

$$EER = \frac{\phi_{tci}}{P_t} \tag{7}$$

$$\phi_{tci} = \sum P_{ic} + (h_{w1} - h_{w2})W_r + \phi_{lp} + \phi_{li}$$
(8)

In Equation 7,  $\phi_{tci}$  refers to the total cooling capacity required on the indoor side, while  $P_t$  describes the total power consumed by the equipment under test. While  $\phi_{tci}$ obtained using Equation 8. The  $P_{ic}$  reflects the total power entering the indoor side test chamber, including lighting power, electrical power consumed by the equipment, and heat generated by compensation and humidification devices;  $h_{w1}$  is the specific enthalpy of water supplied to the indoor side test chamber, while  $h_{w2}$ describes the specific enthalpy of moisture condensed and exiting the chamber.  $P_{ic}$  is the condensation rate of water vapor in the room;  $\phi_{lp}$  describes heat leakage that occurs through partitions that separate the inside of the room from the outside;  $\phi_{li}$  described heat leaks occurring through the walls, floor, and ceiling of an indoor side test chamber (83).

By obtaining comprehensive AC specifications, including electrical power and efficiency factors, this study can continue a more detailed analysis of AC power consumption. The analysis will provide deeper insight into the extent to which the role of fuzzy logic in regulating AC values can affect the power consumption required to maintain room temperature at a certain level.

**2. 4. Energy Consumption Analysis Method** The test was carried out by turning on the AC for 30 minutes using the manual method and the fuzzy method. The calculation of electrical power is measured to obtain energy consumption. During the test, AC power was measured using a watt meter and recorded once every minute. One record per minute is assumed to represent the electrical power used in 1 minute, so to get the electrical power usage for 1 minute is calculated using Equation 9.

$$P_{minute} = P \ x \ 60s \tag{9}$$

In Equation 9, *P* is the electrical power used in 1 second. While  $P_{minute}$  is electrical power used in 1 minute. After getting the electrical power consumption per minute, the next calculated electrical power consumption during the test, which is  $\frac{1}{2}$  hour or 30 minutes. So, to obtain the total use of electrical power within 30 minutes obtained using Equation 10.

$$P_{\frac{1}{2}hour} = \frac{P_{minute} \times 60 \text{ minutes}}{2} \tag{10}$$

Or convert in 1 hour (60 minutes) using Equation 11.

$$P_{hour} = P_{minute} \ x \ 60 \ minutes \tag{11}$$

If you want to convert it in kilowatt-hours (kWh), you can use Equation 12.

$$E_{(kWh)} = \frac{P_{hour}}{1600000} \tag{12}$$

Energy (E) in kWh is equal to power (P) in watts (W), multiplied by the time period t in hours, divided by 1000 as in Equation 13.

$$E_{(kWh)} = \frac{P_{(W)} \times t_{hour}}{1000}$$
(13)

The watt meter used is as in Figure 2.

#### **3. MAIN RESULTS**

3.1. Hypothesis The hypothesis of this study posits that the incorporation of fuzzy logic into room temperature and humidity regulation systems can lead to reduced resource consumption through several means. Firstly, fuzzy logic enables intelligent and adaptive control of temperature and humidity. Utilizing sensors to measure the current temperature and humidity, fuzzy inference systems can make informed decisions regarding whether to activate or deactivate heating or air conditioning devices. This prevents unnecessary energy usage when the temperature or humidity already falls within the desired range. Secondly, by employing linguistic variables and well-defined rules, fuzzy inference systems can finely tune temperature and humidity settings. For instance, if the room temperature is only slightly above the desired threshold, a fuzzy inference system can generate adjustments that proportionally reduce heating or air conditioning power. This mitigates excessive energy consumption associated with traditional ON/OFF methods.

Furthermore, fuzzy logic can take into account other factors influencing the comfort of room occupants. For example, if the external temperature is low but the humidity level is high, a fuzzy inference system can generate settings that slightly raise the temperature and lower the humidity to maintain comfort. By considering humidity, fuzzy inference systems contribute to optimizing overall energy utilization. Additionally, fuzzy

logic enables the scheduling of energy usage based on observed usage patterns. For instance, if room temperature tends to increase during daylight hours, a fuzzy inference system can pre-condition the room by activating the heater or AC beforehand. This approach enhances energy efficiency and prevents excessive energy usage once the desired temperature is reached.

3. 2. Discussion In this experiment, the air conditioner (AC) was operated for a duration of 30 minutes to assess its power consumption. The testing was conducted using two distinct methodologies: the manual approach and the fuzzy logic approach. The manual approach involved direct measurement and calculation of AC power consumption over the 30-minute period. Data for this method were manually recorded from wattage meter readings at 1-minute intervals, which were then used to compute the total AC power consumption. On the other hand, the fuzzy logic approach also recorded electrical power consumption through manual readings from the watt meter, similar to the manual method. However, the fuzzy method utilized a real-time fuzzy logic algorithm to regulate the AC's temperature.

The objective of these tests was to compare the energy consumption of each approach. The test results will yield valuable insights into managing AC power consumption, which can be leveraged for energy conservation and reducing operational costs.

3.2.1. Testing with Manual Method The manual method was assessed by measuring electrical power consumption at various AC temperature setpoints. A total of 8 tests were conducted, with each test performed at a distinct temperature setting: 18°C, 20°C, 23°C, 24°C, 25°C, 26°C, 27°C, and 30°C. Each test spanned 30 minutes to guarantee precise and uniform data collection. The testing procedure is illustrated in Figure 3.

Figure 3 displays the test conducted at an AC temperature setpoint of 25°C. The utilized modes in each test are "Cooling mode" and "Fan mode" both operating concurrently. In each test, data is meticulously recorded at 1-minute intervals based on the watt meter readings to

Fan mode Electric power (per second) Automatic mode AC Temp 25 Celcius

Figure 2. Watt Meter AC Digital Volt

Figure 3. Manual Measurement Process of Electric Power at AC Temperature =  $25^{\circ}C$ 





ensure comprehensive data collection. Variations in AC power consumption at various temperatures can be observed and analyzed. The fluctuations in electrical energy consumption, examined in all manual method tests, are summarized in Figure 4.

Figure 4 displays the results of testing the use of AC within a period of 30 minutes with two different modes, namely "Cooling and fan mode" and "Fan only mode". In this test, the difference in energy consumption in the two modes is very clear. In "Cooling and fan mode", the AC works to reach a set temperature setpoint, while running the fan for air circulation. This mode requires high power because the AC must cool the room by lowering the temperature to the desired setpoint and also maintain air circulation with the help of fans. The test results showed that the highest electrical power per second occurred at an AC temperature setpoint of 20°C, where power consumption reached 447.3 watts. This indicates that the lower the temperature to be achieved, the greater the power required by the AC in this mode. Meanwhile, in "Fan only mode", the AC only functions as a fan without cooling the room. This mode results in much lower electrical power consumption compared to the "Cooling and fan mode" mode. The lowest electrical power occurs at an AC temperature setpoint of 30°C, where the power consumption per second is only 16.6 watts. This is because AC only uses power to run the fan without doing the cooling process, so the power requirement is lower. This test provides conclusions about the impact of using both modes on AC electrical energy consumption. The "Cooling and fan mode" mode is more suitable for achieving lower temperatures, but requires more power. On the other hand, the "Fan only mode" mode is suitable for situations where cooling is not required, and this helps in saving energy.

**3. 2. 1. Testing with Fuzzy Logic Method** Testing with the fuzzy logic method requires several main components: fuzzy variables, fuzzy membership functions, and fuzzy rules. These components are used in three stages in Fuzzy Tsukamoto. Fuzzy variables consist of input and output variables. Input variables are used as input in the form of crisp values and are converted to



**Figure 4.** Fluctuations in Electrical Power Consumption in Each Test on the Manual Method

fuzzy values in the fuzzification stage, while output variables are used in the defuzzification stage as the output of the fuzzy logic in the form of crisp values. The input variables used are room temperature and humidity, while the output variable is the AC temperature.

The selection of room temperature and humidity as input parameters in controlling AC temperature using fuzzy logic is based on physics and human comfort. Temperature affects human comfort and can impact AC efficiency, while humidity is also important because it can affect the feeling of warmth or cold. Proper control of both of these parameters can result in more efficient energy use and maintain indoor air quality.

To apply both of these parameters in fuzzy logic, they are divided into several fuzzy sets. The room temperature variable is divided into five fuzzy sets: Very Cold, Cold, Normal, Hot, and Very Hot. Meanwhile, the humidity variable is also divided into five fuzzy sets: Dry, Normal, Quite Wet, Wet, and Very Wet. On the output variable side, the AC temperature used has a range of 18-32°C, divided into three fuzzy sets: Cold, Normal, and Hot. The temperature curve is shown in Figure 5. The humidity curve is shown in Figure 6, and the AC temperature curve in Figure 7. As for the fuzzy rules with monotonic reasoning, there are a total of 25 rules corresponding to the two input variables, each having five fuzzy sets. The formed fuzzy rules are shown in Figure 8.









Figure 7. AC temperature membership function curve

AC Temp			Humidity						
		Dry	Normal	Quite Wet	Wet	Very Wet			
	Very Cold	Hot	Hot	Hot	Hot	Normal			
Room Temn	Cold	Hot	Hot	Hot	Normal	Normal			
	Normal	Normal	Normal	Normal	Normal	Normal			
	Hot	Normal	Normal	Cold	Cold	Cold			
	Very Hot	Normal	Cold	Cold	Cold	Cold			
Figure 8. Fuzzy rules									

The membership function curves and fuzzy rules in Figures 5-8 are used to control room temperature, which will affect electrical power consumption. This fuzzy method was tested by measuring electrical power consumption on six tests. The temperature setpoint of the AC is not fixed and depends on the temperature and humidity conditions of the room during the test process. Similar to manual method testing, fuzzy method testing is also tested in a duration of 30 minutes in each test. This fuzzy method also presents 2 made air conditioners during the testing process, namely "*Cooling and fan mode*" and "*Fan only mode*". The comparison of AC temperature setpoints to their electrical power consumption is listed in Figure 9.

Figure 9 shows the ratio of AC temperature setpoints to their electrical power consumption in all tests on fuzzy control methods. The value described by the graph of electrical power consumption is taken for 30 minutes at





Electric Power Consumption (Controlled Using Fuzzy Logic)

intervals of 1 minute. This means that the record is taken per minute for 30 minutes. During the testing process, the AC provided action in "cooling and fan" mode and "fan only" mode. A comparison of basic statistics in each mode can be seen in Figure 10.

In Figure 10, there are maximum power test results per second measured on six different tests. These results show that the highest value is reached at 425.6 watts, and this value is obtained when the AC operates in "cooling and fan" mode. The "cooling and fan" mode involves the AC in the process of cooling the room by running a fan for air circulation. Meanwhile, the lowest value in Figure 10 was recorded at 16.1 watts, and this value was obtained when the AC operated in "fan only" mode or only used a fan without cooling the process. In this mode, the AC does not require large power because its function is limited only to running the fan for air circulation without lowering the room temperature. To be able to evaluate each test, the total electrical power in each test using fuzzy control mode is shown in Figure 11.

The total electrical power consumption in Figure 11 is obtained by calculation using Equations 9 and 10. The highest electrical power consumption was obtained in the 3rd test with a consumption of 479347 watts or equivalent to 0.133 kWh (Equation 12). While the most efficient or lowest consumption was obtained in the 5th test with a total electrical power consumption of 98742



**Figure 10.** Comparison of maximum, average, and minimum electrical power in the test with fuzzy logic at (a). fan only mode; and (b). Cooling and fan mode"



Figure 11. Total power consumption in each test with fuzzy logic control

watts or equivalent to 0.027 kWh. If averaged all electrical power consumption in all tests, then a value of 290211 watts or equivalent to 0.081 kWh is obtained. This value is categorized as more efficient when compared to manual methods that tend to consume a lot of electrical power. The results of the comparison between the total electric power consumption of the manual method with the average electric power consumption of the fuzzy method are listed in Figure 12.

Figure 12 shows that the average power consumption using the fuzzy method is lower than most tests on the manual method. Electric power consumption with the fuzzy method is only less efficient than using the



**Figure 12.** Comparison Between the Total Electric Power Consumption of the Manual Method with the Average Electric Power Consumption of the Fuzzy Method

manual method at the AC temperature setpoint =  $30^{\circ}$ C, which is with a difference of 140745 watts (0.039 kWh). While manual control at other AC temperature setpoints (18°C, 20°C, 23°C, 24°C, 25°C, 26°C, and 27°C) consumes much more electrical power when compared to the average power consumption in fuzzy control. The largest difference is in the manual control setpoint of 18°C and followed by the setpoint of 20°C. This is because at setpoints of 18°C and 20°C, the AC works in maximum conditions in "Cooling and fan" mode every second. This makes electrical power consumption also increase. Based on these results, it can also be concluded that electrical power consumption is also influenced by the amount of temperature that AC wants to produce. The smaller the desired temperature, the greater the power required by the AC, so this will make electrical energy consumption higher (84). To see the comparison of the difference in average electrical power consumption between these two methods (manual and fuzzy), it can be seen in Figure 13.

Figure 13 shows that the difference in average energy consumption is quite significant, reaching 209,820.75 watts (0.058 kWh). The average power consumption of the manual method is nearly twice that of the fuzzy method. Energy savings from the use of the fuzzy method amount to approximately 41.96%. A comparison with some previous studies is shown in Table 1.

Table 1 illustrates an interesting comparison across various studies regarding the use of fuzzy logic in controlling AC for energy savings. Different research outcomes show varying degrees of energy savings achievable through this approach. In 2018, a study by



Figure 13. Comparison of the average total electrical power consumption of manual method and fuzzy method

Ref.	Method	Controlled device	Energy savings	Year
(85)	Fuzzy logic	Electronic devices, including the AC	40%	2018
(84)	Fuzzy logic	AC	33.55%	2019
(82)	Fuzzy logic	AC	25%	2020
(27)	Fuzzy logic	AC	62%	2022
(86)	Fuzzy logic	AC	16- 25%	2023
This Research	Fuzzy logic	AC	41,96%	2023

**TABLE 1.** Comparison with some previous studies

Pratama and Sarno (85) on controlling electronic devices, including AC, with fuzzy logic successfully achieved 40% energy savings. Meanwhile, Berouine et al. (84) in 2019 and Shah et al. (82) in 2020 focused on AC control with fuzzy logic, achieving savings of approximately 33.55% and 25%, respectively. However, in 2022, a study by Francis et al. (27) achieved an impressive energy savings of 62% when controlling AC with fuzzy logic. Recent research in 2023 shows varying results, with energy savings ranging from 16% to 25% when controlling AC with fuzzy logic (86).

This study, conducted in 2023, achieved an energy savings of approximately 41.96% when controlling AC using fuzzy logic. A visual comparison of all the literature is shown in Figure 14.

When compared to several previous studies as outlined, this research demonstrates a commendable contribution, trailing behind only the study conducted by Francis et al. (27) with a difference of 20.04%. Nevertheless, these findings already indicate that the application of fuzzy logic in AC control can optimize electrical power usage intelligently by adapting operations to the actual needs of the room and environmental conditions. In the "cooling and fan" mode, the fuzzy method allows for the restriction of AC activity



Figure 14. Comparison of Energy Savings with Previous Studies

when the desired temperature has been achieved or considers room temperature fluctuations to reduce unnecessary power consumption. These results can also serve as a smart solution to reduce energy consumption across various contexts.

#### 4. CONCLUSIONS

The results of this study involved AC running for 30 minutes to observe power consumption by applying two different methods, namely the manual method and the fuzzy method. The manual method involves direct measurement and calculation of AC power used over a 30-minute period by manually recording data from watt meter readings at 1-minute intervals. Meanwhile, the fuzzy method also records electrical power consumption manually, but uses fuzzy logic algorithms to control the temperature of the AC in real-time. The test results show that the fuzzy method is more energy efficient than the manual method, except at a 30°C AC temperature setpoint. The difference is due to the "Cooling and fan" mode used at lower temperatures in the manual method, resulting in higher power consumption. Overall, the average test results of each method indicate that the fuzzy method has a lower average electrical power consumption compared to the manual method, with a significant difference. The use of the fuzzy method can achieve energy savings of approximately 41.96%. This demonstrates the potential of fuzzy methods in optimizing AC power usage in a smarter and adaptive manner based on room and environmental conditions.

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*چکید*ه

#### Persian Abstract

مصرف انرژی یک جنبه حیاتی در تلاش برای استفاده بهینه از منابع و کاهش اتلاف انرژی است. تمرکز بر بهره وری انرژی می تواند منجر به صرفه جویی در هزینه های عملیاتی، کاهش انتشار گازهای گلخانه ای و حمایت از پایداری زیست محیطی برای نسل های آینده شود. بنابراین، توجه به بهره وری انرژی در زندگی روزمره، به ویژه در استفاده از برق برای وسایل الکترونیکی مهم است. هدف این تحقیق مقایسه کارایی انرژی دو رویکرد مختلف برای استفاده از تهویه مطبوع (AC) است: روش دستی و روش منتق برای وسایل الکترونیکی مهم است. هدف این تحقیق مقایسه کارایی انرژی دو رویکرد مختلف برای استفاده از تهویه مطبوع (AC) است: روش دستی و روش منتق فازی. روش دستی شامل هشت آزمایش با اندازه گیری مستقیم توان در یک دوره ۳۰ دقیقهای در تنظیمات مختلف دمای AC، یعنی ۸۸ درجه سانتیگراد، ۲۰ درجه می تعقیق نشان می دهد که روش منطق فازی به جز در دمای منطق فازی به جز در دمای استیگراد که روش دستی گراد است. و ۳۰ درجه سانتیگراد که روش دستی گراد ان در ولی معرفی که در موش درجه سانتیگراد که روش دستی گراد است (تفاوت ۱۹۷۵ و اور) به میانگین توان مصرفی کمتری دست می یابد. این تعاوت در درجه اور مربط به حالت اخنک کننده و فن " است که در درماهای پایین تر در روش دستی استفاده می شود و در نتیجه مصرف برق بیشتر می شود. علاوه بر این، این تعقیق پتانسیل منطق فازی را در سازی مصرفی برق را در درمای پاین می تول در و سی بیشان می در در وش دستی می آورد. سه مسینی می مون برزی که روش در مورد این ولی می تول در ورش دستی می آورد. می مود و در نتیجه مصرف برق بیشتر می شوه بر این این مطالعه ارائه بینش می مورد برزی که روش می مود برزی می تولن به مور قابل توجهی مصرف از ری که را در ان روی ایرژی می توان در یم مواند به مور قابل ت



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### A Comparative Analysis of Axial and Radial Forces in Windings of Amorphous Core Transformers

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#### **1. INTRODUCTION**

The utilization of amorphous material in the magnetic circuits of distribution transformers has gained prominence since its development in 1970s. These transformers, known as amorphous transformers (ATs), have become prevalent in power systems due to their no-load lower losses compared to traditional transformers. This reduction in losses contributes to an overall decrease in the total losses of power systems. The extensive research has demonstrated that the ATs can achieve a significant reduction of 50-70% in no-load losses compared to transformers with silicon steel cores (1-5). Due to the special structure of the steel core and the coil with the rectangular shape of the ATs, the distribution of electric field and forces on the windings will be different on the same turn of the coil. Under the normal operating conditions, the electromagnetic forces (EMFs) acting on the windings are small due to the relatively small magnitude of the leakage flux. However, under the short-circuit condition, the electromagnetic

The aim of this study is to examine and analyze the axial and radial forces, electromagnetic forces (EMFs) acting on the low and high-voltage windings of an amorphous core transformer via the two different approaches: an analytic approach and a 3-D finite element method (FEM). Firstly, the analytic method is proposed to analyze the distribution of leakage magnetic field in the magnetic circuit and the forces acting on the transformer windings. The FEM embedded in the Ansys Maxwell tool is then proposed to compute and simulate the axial and radial forces under three different operating conditions: no-load, rated full-load, and short-circuit. The obtained results from two different methods such as the rated voltage, rated current, short-circuit current, axial and radial forces and EMFs in the low and high-voltage windings are finally compared to illustrate an agreement of methods. The validation of the methods is applied on a three-phase amorphous core transformer of 1600kVA-22/0.4kV.

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forces (EMFs) generated as a result of the interaction between the leakage flux and the short-circuit current are very large, this can lead to translation, destruction, or even explosion of the windings (6-10).

In practices, among various types of transformer faults, winding faults account for approximately 33% of the total occurrences. These faults typically arise from short-circuits between turns within the high voltage (HV) or low voltage (LV) windings, between different layers of windings, between HV and LV windings, or even between phases within the same winding. In such cases, the resulting EMFs or mechanical forces (MFs) can cause bending or destruction of the transformer windings (11-16). The EMF can be further categorized into two distinct components: axial force (Fx) and radial force (Fy). The Fx generated by the interaction between the current in the winding and the axial magnetic field (By) is perpendicular to the winding axis. On the other hand, the Fy produced from the interaction between the current in the winding and the horizontal magnetic field (Bx), is parallel to the winding axis (17-22).

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Wang et al. (7) provided a detailed description of the design and operation of a three-phase AT with a capacity of 630 kVA-10.5/0.4 kV. The study focused on acquiring the fundamental characteristics of the AT through standard short-circuit and no-load tests. The utilization of amorphous alloy as the iron core material in the AT offers several advantages, including reduced losses and excellent magnetization characteristics. Consequently, amorphous alloys have found widespread application in small-capacity distribution power transformers.

Zhong et al. (8) used a finite element method (FEM) to compute the stress and strain of the end covers and the winding clamps of the AT of 800 kVA/10 kV. Based on that, the shell-form transformer demonstrated the superior capability to withstand short-circuits, and historical evidence has primarily relied on the use of silicon steel iron core materials. Kumbhar and Kulkarni (23) analyzed the EMFs acting on the windings of splitwinding transformers by using a nonlinear-transient field-circuit coupled finite element model. In this study, a three-phase split-winding transformer of 70MVA-220/3.6/6.9kV was simulated and examined via the FEM under both preset and postset short-circuit test conditions. Mouhamad et al. (24) conducted the short-circuit withstand tests of Metglas 2605SA1-based amorphous transformers, rated 240 to 630kVA. In this paper, the authors focused on calculating the short-circuit current and the electrodynamic forces experienced by the transformer windings. However, their work did not explicitly address the distribution of the leakage magnetic field or the axial and radial forces within the transformers. Bal et al. (25) used the FEM embedded in ANSYS Maxwell simulation program to analyze the electromagnetic transients and compute the losses, voltages, currents and magnetic fluxes of a three-phase oil-type distribution transformer with a capacity of 25kVA. Li et al. (26) presented the distribution of EMF in a three-phase power transformer of a 50MVA/110 kV under short-circuit conditions via the FEM. Jin et al. (27) explored the stress distribution characteristics of a composite wire-paper winding structure when subjected to radial electromagnetic forces. A copper-paper layered ring was employed as the experimental setup. The study involved calculating both the hoop stress distribution and the radial stress distribution within the winding structure. The FEM was then used to verify the obtained results. Zhai et al. (28) established a three-dimensional model of the transformer to investigate the electrodynamic force and deformation of transformer windings under shortcircuit conditions. The distribution transformers have received limited attention in previous studies, with few investigations conducted on this specific type of transformer. Furthermore, the existing literature lacks a comprehensive model for calculating Fx and Fy in distribution transformers. However, in literature review (29-32), the FEM is employed to analyze and compute various parameters such as leakage magnetic field, leakage reactance, and electromagnetic forces in both the HV and LV windings of the transformer during shortcircuit tests. In these studies, a mathematical model was proposed to calculate the current and transient electromagnetic force. The leakage magnetic field density and average electromagnetic force were provided based on FEM simulation results. These obtained results using FEM are then compared with those of the analytic method.

The EMFs can be calculated by using different methods. The analytic method can provide a comprehensive and faster solution. Unfortunately, these methods may not be applied in models with nonlinear materials, complex geometric structures, and/or boundary conditions. Therefore, the FEM method based on Ansys Maxwell 3D software in the time domain is applied to solve the problem with complex shapes, multiphysics environment, and the EMFs calculation in each part or each position of the windings. Thanh et al. (33) used 2D FEM to analyze and calculate the magnetic field for a 160kVA indefinite shape MBA. In this paper, the model is considered in a short-circuit mode with maximum current, without considering the 3D model under various operating conditions such as no-load, rated load, and three-phase short-circuit conditions on the lowvoltage side.

In general, as mentioned above, the FEM to analyze and calculate the distribution of magnetic fields, fringing and leakage impedances and electromagnetic forces acting on the HV and LV windings of the MBA in shortcircuit conditions. They also provided formulas to calculate the overcurrent and electromagnetic force during short-circuit conditions. The results obtained include 2D FEM images of the magnetic field density and average electromagnetic forces, which are then compared with classical analytical methods. Furthermore, there are very few research works on the magnetic field and electromagnetic force of the armorphous steel-core MBA. No research has comprehensively analyzed and evaluated various operating conditions of the armorphous MBA using 3D FEM models, progressing from analytical models to full 3D FEM models. Using a 3D FEM model approaches a nearly real representation of the MBA, allowing for the analysis of multi-physics phenomena, including mechanical, electrical, and thermal effects. This approach helps accurately to determine the winding strength in various short-circuit condition, which can be challenging to achieve through analytical methods and experiments.

Based on the development from published paper by Thanh et al. (33), in this context, the magnetic vector potential. Formulations (A) is first presented to define the distribution of leakage magnetic field in the magnetic circuit and the distribution of EMFs in the transformer windings. Then, the FEM is developed based on Ansys Maxwell 3D in the time domain to simulate electromagnetic parameters of a three-phase TA of 1600kVA, 22/0.4 kV under several operating conditions, such as no-load, rated full-load and short-circuit. The obtained results from the FEM are verified and compared with the analytic model in terms of accuracy. In addition, the EMFs acting on the HV and LV windings will be also determined in the case of a three-phase short-circuit of the LV winding. This research is conducted based on the following assumptions: (1) the neglect of eddy current effects in the windings; (2) the assumption of uniform current density in the windings; (3) the consideration of a symmetric model for analysis.

# 2. SHORT-CIRCUIT ELECTROMAGNETIC FORCE ANALYSIS

**2. 1. Short-circuit Current** The short-circuit current flowing in the windings has the potential to cause damage to the transformer windings. This transient short-circuit current comprises two different components, namely (8, 29, 34):

$$i_{SC} = i_{hos} + i_{dos}$$
  
=  $I_n \sqrt{2} . \sin(\omega t - \phi - \phi_n) + I_n \sqrt{2} . \sin(\phi + \phi_n) . e^{-\frac{R_n}{X_n} \omega t}$  (1)

where:

- i<sub>hos</sub> is the harmonic oscillation,

- i<sub>dos</sub> is the damped oscillation,

-  $I_n = \frac{U_{rated}}{Z_n}$  is the root mean square (SMS) of short-circuit

current (A),

-  $\varphi_n = \operatorname{arctg} \frac{X_n}{R_n}$  is the phase angle (rad),

- Urated is the rated voltage

-  $Z_n$  is the short-circuit impedance ( $\Omega$ ),

-  $X_n$  and  $R_n$  are respectively short-circuit resistance and reactance ( $\Omega$ ),

- t is the time (s),

-  $\phi$  is the angle depending on the short-circuit time (rad), -  $\omega$  is the angular frequency (rad/s).

2. 2. Analytic Model for Computation of the Leakage Magnetic Fields and EMFs in Transformer Windings Based on Maxwell's equations, the separate equation for the stationary electromagnetic field  $(\partial/\partial t = 0)$  in the transformer windings associated with the current density J, the Laplace-Poisson's equation for A(x,y,z) can be obtained as follows (22, 26, 28, 33):

$$\nabla^{2} \mathbf{A}(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \begin{cases} -\mu \mathbf{J} & \text{in the windings} \\ 0 & \text{others} \end{cases}$$
(2)

In three-dimensional Descartes coordinates, Equation 2 can be written as:

$$\frac{\partial^2 \mathbf{A}(\mathbf{x}, \mathbf{y}, \mathbf{z})}{\partial x^2} + \frac{\partial^2 \mathbf{A}(\mathbf{x}, \mathbf{y}, \mathbf{z})}{\partial y^2} + \frac{\partial^2 \mathbf{A}(\mathbf{x}, \mathbf{y}, \mathbf{z})}{\partial z^2} = -\mu \mathbf{J}$$
(3)

where A(x,y,z) is the magnetic vector potential,  $\mu$  is the relative permeability (H/m) and J is the electric current density in the windings (A/m<sup>2</sup>).

In Figure 1, the magnetic field is perpendicular to the plane  $(\partial A/\partial z = 0)$ . Hence, Equation 3 can be represented as:

$$\frac{\partial^2 \mathbf{A}(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}^2} + \frac{\partial^2 \mathbf{A}(\mathbf{x}, \mathbf{y})}{\partial \mathbf{y}^2} = -\mu \mathbf{J}$$
(4)

where the **J** can be computed via the electric current density in the HV winding  $(\mathbf{J}_1)$  and LV winding  $(\mathbf{J}_2)$ , that is:

$$\mathbf{J}_{1} = \frac{\mathbf{W}_{1} \mathbf{i}_{1}}{\mathbf{a}_{1} \mathbf{b}_{1}}; \mathbf{J}_{2} = \frac{\mathbf{W}_{2} \mathbf{i}_{2}}{\mathbf{a}_{2} \mathbf{b}_{2}}$$
(5)

where  $a_1b_1$  and  $a_2b_2$  are the cross-sections of the HV and LV windings, respectively. The quantities  $i_1$  and  $i_2$  are the electric currents in HV and LV windings, respectively. The magnetic vector potential **A** (x,y) in Equation 4 can be analysed in the form of a harmonic series:

$$\mathbf{A}(\mathbf{x}, \mathbf{y}) = \sum_{j} \sum_{k} A_{j,k} \cos(m_j \mathbf{x}) . \cos(n_k \mathbf{y})$$
(6)

where  $A_{j,k}$  is the constant of integration calculation. The terms of m and n are the phase angles.

The components of a magnetic field in the x- and yaxis at the boundaries of the magnetic window are



Figure 1. Typical dimensions of windings and the magnetic circuit

(8)

considered as a zero (i.e.,  $B_x = 0$  and  $B_y = 0$ ). The boundary conditions (BCs) are defined as:

$$\sin(\mathbf{m}_{j}\mathbf{d}) = \mathbf{0} \to \mathbf{m}_{j} = (j-1)\frac{\pi}{\mathbf{d}}$$
(7)

$$\sin(n_k h) = 0 \rightarrow n_k = \left(k - 1\right)\frac{\pi}{h}$$

where j and k are the integers.

For j = k = 1 and  $m_1 = n_1 = 0$ , the harmonic sequence is a constant. The constant of integration  $A_{j,k}$  can be generally illustrated as:

$$\begin{split} A_{j,k} &= \frac{4 \, \mu_0}{d.h} \frac{1}{m_j n_k (m_j^2 + n_k^2)} \times \\ & \left[ J_1 \left( sinm_j d_2^1 - sinm_j d_1^1 \right) \left( sinn_k h_2^1 - sinn_k h_1^1 \right) \\ & + J_2 \left( sinm_j d_2^2 - sinm_j d_1^2 \right) x \left( sinn_k h_2^2 - sinn_k h_1^2 \right) \right] \end{split} \tag{9}$$

The magnetic flux density (**B**) can be given as  $\mathbf{B} = \nabla \times \mathbf{A}$ , the components of **B** in the x- and y- axis at the boundaries of the magnetic window are expressed as:

$$\begin{cases} \mathbf{B}_{x} = \frac{\partial \mathbf{A}(x, y)}{\partial y} \\ \mathbf{B}_{y} = -\frac{\partial \mathbf{A}(x, y)}{\partial x} \end{cases}$$
(10)

**2.3. The Axial and Radial Forces in the Windings** As presented, the EMFs acting on the transformer windings are the interaction between the transient currents and the leakage magnetic field within the winding regions. For that, the EMF can be split into two components, i.e., the  $F_x$  and  $F_y$  as shown in Figure 2. The observed trends of these forces are as follows:

- They exert compression forces, leading to a reduction in the radius of the inner coil.
- They exert tension forces, resulting in an increase in the radius of the outer coil.
- They exert compression forces, causing a decrease in the height of both coils.



**Figure 2.** Components of magnetic induction field Fx and Fy in the transformer windings

\* The components of EMF in the LV winding, per unit length of the winding:

The radial force  $(F_{X-LV})$  in the x-axis is defined as:

$$F_{X_{LV}} = \int_{d_1^1 h_1^1}^{d_2^1 h_2^1} J_I B_y dx \, dy = -J_I \int_{d_1^1 h_1^1}^{d_2^1 h_2^1} \frac{\partial \mathbf{A}(x, y)}{\partial x} dx \, dy$$
(11)

In the same way, the radial force  $(F_{y\text{-}LV})$  in the y-axis is defined as:

$$F_{Y_{\perp}LV} = \int_{d_1^1 h_1^1}^{d_2^1 h_2^1} J_1 B_x dx \, dy = J_1 \int_{d_1^1 h_1^1}^{d_2^1 h_2^1} \frac{\partial \mathbf{A}(x, y)}{\partial y} dx \, dy$$
(12)

\* The components of EMF in the HV winding, per unit length of the winding:

The radial force  $(F_{X-HV})$  in the x-axis is defined as:

$$F_{X_{L}HV} = \int_{d_1^2 h_1^2}^{d_2^2 h_2^2} J_2 B_y dx \, dy = -J_2 \int_{d_1^2 h_1^2}^{d_2^2 h_2^2} \frac{\partial \mathbf{A}(x, y)}{\partial x} dx \, dy$$
(13)

In the similar way, the radial force  $(F_{y-HV})$  in the y-axis is defined as:

$$F_{Y_{-HV}} = \int_{d_1^2 h_1^2}^{d_2^2 h_2^2} J_2 B_x dx \, dy = -J_2 \int_{d_1^2 h_1^2}^{d_2^2 h_2^2} \frac{\partial \mathbf{A}(x, y)}{\partial y} \, dx \, dy$$
(14)

### **3. ANALYTICAL TEST**

The practical test problem is a three-phase amorphous core transformer of 1600kVA-22/0.4kV produced by the Sanaky transformer manufacturing factory as depicted in Figure 3. The parameters are given in Table 1. The cross-section of the core is the rectangular with the magnetic tape width b = 170 mm, thickness 2b = 340 mm; circuit window height H<sub>cs</sub> = 550 mm, and distance between two cylinder centers Mo = 435 mm.

The short-circuit currents in the HV and LV windings are illustrated in Figures 4 and 5, respectively. The maximum short-circuit currents in the HV and LV windings are shown in Table 2.



Figure 3. Model of a three-phase 1600kVA-22/0.4kV

**TABLE 1.** Basic parameters of a three-phase amorphous core transformer

No.	Parameter	Value
1	No. of phases	3
2	Frequency [Hz]	50
3	Capacity [kVA]	1600
4	Wiring connections	Δ/Y-11
5	Hv/LV [kV]	22/0.4
6	Turns of HV/LV windings	1001/10
7	Phase current in HV/LV windings [A]	24.24/2309.4
8	Short-circuit current in HV/LV windings [A]	542.28/51664.43



Figure 4. Distribution of the short-circuit current in the HV winding

**TABLE 2.** Maximum short-circuit currents in the HV and LV windings

Parameter	LV winding	HV winding
Maximum short-circuit current (A)	111090	1102.8

Based on Equation 5, the electric current densities in the LV and HV windings can be respectively calculated as:

$$J_{1} = J_{nLV} = \frac{W_{LV}i_{nLVmax}}{a_{1}b_{1}}$$

$$= \frac{10 \times 111090}{23 \times 520} \times 10^{6} = 92.88 \times 10^{6} (A / m^{2})$$
(15)

$$J_{2} = J_{nHV} = \frac{W_{HV} i_{nHVmax}}{a_{2}b_{2}}$$

$$= \frac{1001 \times 1102,8}{37 \times 520} \times 10^{6} = 57.38 \times 10^{6} (A / m^{2})$$
(16)

By using the MATLAB software, the magnetic vector potential **A** is demonstrated in Figure 6.

From Equations 11 to 14, the  $F_x$  and  $F_y$  in the LV winding are pointed out in Figures 7 and 8, respectively.

In Figure 7, it can be seen that the LV winding along the y-axis (height of winding) is pushed inwards by the  $F_x$ . The distribution of this force gradually diminishes towards the two ends of the winding. The maximum value of the radial force occurs at the middle of the winding, reaching a peak value of  $F_{xmax} = 24.94.10^7$  N/m<sup>2</sup>.



Figure 5. Distribution of the short-circuit current in the LV winding



Figure 6. Distribution of magnetic vector potential



Figure 7. Radial force (F<sub>x</sub>) in the LV winding

Figure 8 illustrates that the distribution of  $F_y$  is predominantly concentrated at the two ends of the winding, with a maximum value of  $F_{ymax} = \pm 1.862 \times 10^7 \text{N/m}^2$ . In contrast, the  $F_y$  becomes zero at the midpoint of the winding.

The distribution of  $F_x$  along the y-axis (height of winding) of the HV winding is presented in Figure 9. It shows that the LV winding is pushed far away. The distribution of this force gradually decreases to the two ends of the winding. The maximum value of radial force is at the middle of the winding with  $F_{xmax} = -15.44 \times 10^7 N/m^2$ . In the same way, the distribution of  $F_y$  is given in Figure 10. It can be seen that this force concentrates at the two ends of the winding with the maximum value of  $F_{ymax} = \pm 3.31 \times 10^7 N/m^2$ . It becomes zero in the middle of the winding. The maximum EMFs acting on the HV and LV windings are represented in Table 3.

#### 4. NUMERICAL TEST

An analytic test was given in the previous Section, in this section, the FEM is applied to verify the results from the analytic model. Keep the same prameters of the



Figure 8. Axial force (F<sub>y</sub>) in the LV winding



Figure 9. Radial force (F<sub>x</sub>) in the HV winding



Figure 10. Axial force (Fy) in the HV winding

TABLE 3. Maximum EMFs acting on the HV and LV windings

Maximum force (10 <sup>7</sup> ) (N/m <sup>2</sup> )	LV winding	HV winding
F <sub>xmax</sub>	24.94	-15.44
Fymax	$\pm 5.35$	$\pm 3.31$

amorphous core transformer of 1600kVA - 22/0.4kV given already in Figure 1 and Table 1. The steel code of 2605HB1M has the magnetic induction field B = 1.63T. The amorphous core is pointed out in Figure 11. The geometry of the steel core generated in Ansys Maxwell 3D given in Figure 12. To minimize the calculation time, half of the cross-section in 3D is utilized due to the model inherent symmetry. In addition, the insulation material and support structure are neglected in this model (31).

The algorithm for calculation of the  $F_x$  and  $F_y$  using Ansys Maxwell 3D in different operating conditions is proposed in Figure 13.

The simulation test includes three different operating conditions: no-load, rated full-load, and short-circuit. The time intervals for each condition are as follows:

- Firstly, the no-load condition is simulated from 0 to 50 ms
- Secondly, the rated full-load condition is simulated from 50 to 100ms



Figure 11. Steel core of the three-phase amorphous core transformer



Figure 12. Geometry of the steel core generated in Ansys Maxwell 3D



Figure 13. Algorithm for computation of Fx and Fy using Ansys Maxwell 3D

• Finally, the short-circuit condition is simulated from 150 ms to 300ms.

Figure 14 illustrates the distribution of B in the steel core of at a specific time t = 56ms.

The investigation focuses on the value and direction of the magnetic field in the magnetic circuit under both no-load and rated full-load conditions. In this analysis, the maximum magnetic flux density achieved is  $B_{max} =$ 1.78T. Subsequently, the study examines the voltages and currents in the windings of the AT, as follows.

4. 1. Under the Rated Full-load Condition The three-phase rated voltage in HV and LV windings are



Figure 14. Distribution of magnetic flux density (B) at t = 56ms

shown in Figures 15 and 16, respectively. According to Figure 15, the simulated value of the rated voltage in the HV winding is 311320V (with a calculated value of 31112.7V. Similarly, as illustrated in Figure 16, the simulated value of the rated voltage in the LV winding is 310.7V (with a calculated value of 326.6V). The maximum error between the simulated and calculated values is 4.9%.

The three-phase rated currents in the HV and LV windings is presented in Figures 17 and 18. In Figure 17, the simulated value of the rated current in the HV winding is 33.22A (compared to a calculated value of 34.28A), whereas the simulated value of the rated current in LV winding is 3274.14A (compared to a calculated value of 3265.99A in Figure 18. The maximum error



Figure 15. Three-phase rated voltage in the HV winding



Figure 16. Three- phase fated voltages in the LV winding



Figure 17. Three- phase rated currents in the HV winding



between the simulated and calculated values is 3.1%. The values obtained for voltages and currents using the simulation method align closely with the values derived from the analytic method under both no-load and rated full-load conditions.

#### 4.2. Under the Short-circuit Condition

#### \*) Short-circuit current

The short-circuit test of the LV winding is performed in a three-phase configuration, controlled by switch S as shown in Figure 19. The short-circuit test is initiated at t = 150ms. At this specific time, the voltage in phase B becomes zero, while the short-circuit current in phase B reaches its maximum value. The simulation is then conducted up to 300ms, with an incremental time step of  $\Delta t = 0.1 \text{ms}$ 



Figure 19. Diagram of control circuit

\*) Distributions of leakage magnetic field and electromagnetic forces

The problem is considered in the time domain, allowing for the analysis of the magnetic induction distribution within the magnetic circuit and windings at various operating times of the AT. Specifically, during the shortcircuit period, the currents, magnetic field, and electromagnetic forces in the windings are examined at the time when the short-circuit current reaches its maximum value. Figure 20 illustrates the simulated magnetic induction at t = 159ms during the short-circuit condition.

At t = 159ms, which corresponds to the maximum short-circuit current in phase B, the leakage magnetic field within the winding intensifies to B = 2.6T, while the magnetic induction within the magnetic circuit decreases. A significant portion of the distributed leakage magnetic field is concentrated in the region between the HV and LV windings. Figures 21 and 22 showcase the shortcircuit currents within the HV and LV windings, respectively.

As depicted in Figure 21, at t = 159ms, the shortcircuit current in the HV winding of phase B reaches its maximum value, with I<sub>CA\_max</sub> = 1109.4A. This value is 33 times greater than the rated phase current. Similarly, Figure 22 demonstrates that at t = 159 ms, the shortcircuit current in the LV winding of phase B attains its maximum value, with I<sub>HA\_max</sub> = 111076A. This value is



Figure 20. Magnetic induction at the time of t = 159ms



Figure 21. Short-circuit currents in the HV winding



**TABLE 4.** Comparion of the currents and voltages between the analytic method and FEM

Condition	Winding	Analytic method	FEM	Error %
Ratedphase voltage	HV	31112.7	31120	0.02
(V)	LV	326.6	310.7	4.9
Rated phase current	HV	34.28	33.22	3.1
(A)	LV	3265.99	3274.14	0.2
Short-circuit	HV	1102.8	1109.4	0.6
impulse current (A)	LV	111090	111076	0.01

34 times greater than the rated phase current. Table 4 presents a comparison of the currents and voltages in the HV and LV windings obtained through both the analytic method and the simulation method.

Based on the comparison results presented in Table 4, there are differences between the values obtained using the two methods. It should be noted that these disparities arise because the insulation material and support structure of the AT were disregarded in the model used for this analysis.

**4. 3. EMFs Acting on the HV and LV Windings** The FEM embeded in Ansys Maxwell tool is proposed to analyze both the direction and magnitude of the magnetic field vector surrounding the winding space, as well as the maximum current density during short-circuit conditions. This enables the determination of the distributions of EMFs acting on the HV and LV windings.

At the cross-section of transformer in the Oxy plane, the EMFs can be divided into two components, i.e.,  $F_x = B_y$ .  $J_z$  and  $F_y = B_x$ .  $J_z$ .

The distributions of  $F_x$  and  $F_y$  in the LV winding at the time t = 159 ms are shown in Figure 23 and Figure 24.

As depicted in Figure 23, the  $F_x$  reaches its maximum value at the midpoint of the winding, with  $F_{xmax\_LV} = 24.10 \times 10^7 \text{N/m}^2$  for the LV winding. Similarly, in Figure 24, the  $F_y$  attains its maximum values at the two ends of

the winding, with  $F_{ymax\_LV} = \pm 5.46 \times 10^7 N/m^2$  for the LV winding.

Similarly, the distributions of  $F_x$  and  $F_y$  in the HV winding at the time t = 159ms are pointed out in Figures 25 and 26.

In Figure 25, the  $F_x$  gets the maximum value at the middle of the winding with  $F_{xmax\_HV} = -15.76 \times 10^7 \text{N/m}^2$ , whereas the  $F_y$  gets the maximum values at the two ends of the winding  $F_{ymax\_LV} = \pm 3.39 \times 10^7 \text{N/m}^2$  in Figure 26. The maximum values of  $F_x$  and  $F_y$  and in the HV and LV windings between two methods are given in Table 5.

The maximum total  $F_x$  is concentrated at the center between the outer boundary of the LV winding and the





**TABLE 5.** Comparative results of the maximum values of  $F_x$  and  $F_y$  between two different methods

Winding	$\begin{array}{c} F_{max}\!\!\times\!\!10^7 \\ (N\!/\!m^2) \end{array}$	Analytic method	FEM 3D	Error (%)
I V	F <sub>xLVmax</sub>	24.94	24.10	3.37
Lv	F <sub>yLVmax</sub>	$\pm 5.35$	$\pm 5.46$	2.05
HV	F <sub>xHVmax</sub>	- 15.44	- 15.76	2.07
	F <sub>yHVmax</sub>	$\pm 3.31$	± 3.39	2.41

inner boundary of the HV winding. This force exerts a pulling effect on the winding. The maximum force, as presented in Table 5, is  $F_{xmax} = 24.94 \times 10^7 \text{N/m}^2$ . If the winding is considered as a solid object, the allowable stress for copper is typically within the range of  $\sigma_{safe \ stress} = (5 \div 10) \times 10^7 \text{N/m}^2$  (15). Consequently, when a short circuit occurs with the maximum current, the maximum stress on the winding exceeds the permissible limit.

### **5. CONCLUSIONS**

In this study, a mathematical model based on Maxwell's equations is introduced, enabling the derivation of Laplace-Poisson's equation for the magnetic vector potential formulation. Using this equation, the F<sub>x</sub> and F<sub>y</sub> acting on the windings of the AT of 1600kVA - 22/0.4kV have been successfully calculated. Additionally, the FEM, employing Ansys Maxwell 3D software based on Transient magnetic, is utilized to compute and simulate magnetic flux density and forces under three operating conditions: no-load, rated full-load. After that, it was confirmed that the FEM 3D simulation model was accurate, and researched the short circuit on the LV winding to find maximum the short circuit current; maximum radial and axial electromagnetic force. The obtained values of currents and voltages during rated fullload and short-circuit conditions are compared. The comparison results show that the mathematical modeling and 3D FEM completely coincide. This force may exceed the allowable limit for the winding, thereby risking its

destruction, breakage, or displacement during a short circuit. Use the 3D FEM model to research and calculate and simulate the working modes of the transformer and the short circuit and destructive fault modes that experimental methods cannot do.

For future research, it is suggested to further employ the FEM based on Ansys Maxwell 3D software to investigate the distributions of EMFs at various positions in the windings. The simulation of the AT to determine the maximum force in the windings is crucial for the design, manufacturing, testing, and operation of energysaving amorphous transformers.

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### Persian Abstract

#### چکیدہ

هدف از این مطالعه بررسی و تجزیه و تحلیل نیروهای محوری و شعاعی، نیروهای الکترومغناطیسی (EMF) است که بر روی سیمپیچهای ولتاژ پایین و ولتاژ بالا یک ترانسفورماتور هسته آمورف از طریق دو رویکرد مختلف: یک رویکرد تحلیلی و یک روش محدود سه بعدی تأثیر میگذارند. روش عنصر (FEM). در مرحله اول، روش تحلیلی برای تجزیه و تحلیل توزیع میدان مغناطیسی نشتی در مدار مغناطیسی و نیروهای وارد بر سیم پیچ ترانسفورماتور پیشنهاد شده است. سپس FEM تعبیه در ابزار Ansys Maxwell برای محاسبه و شبیه سازی نیروهای محوری و شعاعی تحت سه شرایط عملیاتی مختلف پیشنهاد می شود: بدون بار، بار کامل نامی و اتصال کوتاه. نتایج بهدست آمده از دو روش مختلف مانند ولتاژ نامی، جریان نامی، جریان اتصال کوتاه، نیروهای محوری و شعاعی و AMS در سیمپیچهای ولتاژ پایین و بالا در نهایت برای نشان دادن توافق روشها با یکدیگر مقایسه می شوند. اعتبار سنجی روش ها بر روی یک ترانسفورماتور هسته آمورف سیمپیچهای ولتاژ پایین و بالا در نهایت برای نشان

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