

International Journal of Engineering

Journal Homepage: www.ije.ir

Chemical Reaction-Diffusion Model Around a Vessel for Studying Temperature and Concentration of Three Chemical Species by Finite Element Method

P. Pasha*a, F. Taghiniab, F. Nadalinia Charib, B. Jalilic, P. Jalilic, D. Domiri Ganjib

- ^a Department of Mechanical Engineering Mazandaran University of Science and Technology, Babol, Iran
- ^b Department of Mechanical Engineering Noshirvani University of Technology, Babol, Iran
- ^c Engineering, Faculty of Engineering, North Tehran Branch, Islamic Azad University, Tehran, Iran

PAPER INFO

Paper history: Received 06 September 2022 Received in revised form 11 October 2022 Accepted 12 October 2022

Keywords: Finite Element Method Chemical Reaction Diffusion Arrhenius Equations

ABSTRACT

In this paper, the temperature and concentration of species around a vessel using the reaction and diffusion relations were investigated. The reactions between 3 chemical species, and the relationship between temperature changes and the rate of chemical reactions were studied. The novelty of this paper is the use of different coefficients of material with diffusion constants and also considering the concentration and temperature of materials involved in the reaction with non-heat sources and with heat source modes. So that showed the concentration and heat transfer rate of substances involved in the chemical reactions in the form of two-dimensional and three-dimensional diagrams about their distance from the borders of the vessel. The finite element method is utilized for calculated differential equations. According to the results obtained, when the temperature of the reactants increased more heat is released; the concentration also changed a lot, and its amount increased. However, in products such as substance (c), it has an inverse relationship with reactants (a) and (b) in such a way that as the concentration and temperature of the reactants increased, these values decreased in the product. On average, concentration changes in the distance from the center to the surroundings the maximum heat source mode was about 76% less than the average heat source mode and about 14% less than the non-heat source mode.

doi: 10.5829/ije.2023.36.01a.19

NOMENCLATURE						
Kt	diffusivities	Н2	Activation energy/k for C			
K_a	diffusivities	a0, b0, c0	Initial distribution			
K_b	diffusivities	T	Temperature			
K_I	Reaction coef for A+B	Q	Heta transfer			
H1	Activation energy/k for A+B	A,B,C	Chemical component			
<i>K</i> 2	Reaction coef for C	C	Concentration			

1. INTRODUCTION

Reaction-diffusion frameworks are scientific models which compare to a few physical marvels. The foremost common is the alteration in space and time of the concentration of one or more chemical substances: neighborhood chemical responses in which the substances are changed into each other, and dissemination which causes the substances to spread out over a surface in space. Reaction-diffusion frameworks

are connected in chemistry. In any case, the framework can portray dynamic forms of non-chemical nature. Cases are found in science, geography, material science (neutron dissemination hypothesis), and biology. Waqas [1] studied the recreation of changed nanofluid demonstrated within the stagnation locale of cross liquid by the expanding-contracting barrel. Farooq et al. [2] investigated the transport of half-breed sort nanomaterial in the peristaltic movement of thick liquid considering nonlinear radiation, entropy optimization, and slip

Please cite this article as: P. Pasha, F. Taghinia, F. Nadalinia Chari, B. Jalili, P. Jalili, D. Domiri Ganji, Chemical Reaction-Diffusion Model Around a Vessel for Studying Temperature and Concentration of Three Chemical Species by Finite Element Method, *International Journal of Engineering, Transactions B: Applications*, Vol. 33, No. 11, (2020) 171-181

^{*}Corresponding Author Email: pasha.pooya@yahoo.com (P. Pasha)

impacts. This article examines entropy optimization in cross-breed nanomaterial streams through turning peristaltic channel dividers. Waqas [3] examined the scientific and computational system for warm exchange investigation of a ferromagnetic non-Newtonian fluid subjected to heterogeneous and homogeneous responses. Wagas [4] considered the chemical response effect in double-diffusive non-Newtonian fluid highlighting variable liquid thermo-solute traits. This thinks about focuses on a two-dimensional rate sort Maxwell fabric stream designed by a vertical moving surface. Warm source/sink and variable conductivity properties are included in vitality expression. Waqas et al. [5] investigated the nonlinear scientific examination of thermally radiative stratified nano liquid, including the perspectives of the attractive field, Robin conditions, and warm radiation. Waqas [6] studied the Dissemination of stratification-based chemically responsive Jeffrey fluid, including blended convection. The rate of heat-mass exchange is taken note higher when stratification factors are expanded because an increase in stratification factors yields lower solute and warm areas. Wagas et al. [7] researched the expository assessment of Oldroyd-B nano liquid beneath thermo-solute Robin conditions and stratifications. Wagas et al. [8] examined the Gyrotactic bioconvection stratified stream of magnetized micropolar nano liquid arranged by stretchable emanating surface with Joule warming and thick dissemination. Guedri et al. [9] considered the warm angles of attractively driven micro-rotational nanofluid designed by exponential emanating sheet. To accomplish such points, nanoparticle-based dispersed fluids may be utilized as working fluids instead of standard fluids to reinforce sunpowered vitality acknowledgment. Waqas et al. [10] investigated the transport of chemically receptive thixotropic nanofluid stream by convectively warmed permeable surface. Ebermann et al. [11] researched the expository and numerical approach to decide compelling dissemination coefficients for composite weight vessels. Shadman et al. [12] studied the combined septum and chamfer balances on threated extending surface beneath the impact of nanofluid and the attractive parameters for revolving seals in computer equipment. In this paper, the variety of temperature and speed within the x-direction and the precise speed of the nanofluids stream through triangular and rectangular, and chamfer fins were examined within the presence of a uniform, attractive field. Fathollahi et al. [13] reviewed the application of numerical and computational strategies to explore the changes within the liquid parameters of the liquid passing over blades of distinctive shapes with the limited component strategy. Abdollahzadeh et al. [14] reviewed the studying the half-breed of radiation and attractive parameters on Maxwell fluid with TiO2 nanotube impact of distinctive edges. Pasha and Domiri-Ganji [15] examining the crossover examination of micropolar ethylene-glycol nanofluid on extending surface mounted triangular, rectangular, and chamfer blades by FEM technique and optimization with RSM strategy. Darezereshki et al. [16] studied the chemical handle of synthesizing zinc oxide (ZnO) with nanorod and circular morphologies. The response temperature of all steps amid the blend of ZnO nano powders moved to a higher temperature as the pH of the beginning arrangement expanded from 6 to 11. Due to the effortlessness, the display strategy can be proposed as a helpful way to deliver unadulterated ZnO nanoparticles utilizing ZnSO₄ and ZnCl₂ arrangements without utilizing any harmful and natural chemicals. Wang et al. [17] investigated the numerical examination of the heat-fluid characteristic interior high-speed precise contact ball bearing greased up with oil. Madani et al. [18] researched the A sequencebased solvency indicator made with widened press excitation leftover systems.

Kunkel et al. [19] investigated the Modeling coronavirus spike protein flow: suggestions for immunogenicity and safe elude. Hosseini et al. [20] reviewed the creation of an Al/Mg bimetallic thin-walled ultrafine-grained tube by extreme plastic distortion diary of materials building and execution. Alrwashdeh et al. [21] investigated the effect of turbocharger compression ratio on performance of the spark-ignition internal combustion engine. The present study is the use of a series of chemically coupled fluid equations that, by using the relationships between them and changes in a series of chemical parameters in software called FlexPDE, were able to study the concentration of reactants and products and also with changes in heat transfer to the center examined the shape of the vessel, the temperature in different areas of the vessel, and showed the heat flux at the boundaries. Also, the relationships between concentration and temperature and the relationship between reaction rate and these factors were investigated. The purpose and necessity of this research are that while getting acquainted with the effect of chemical reactions on concentration and temperature and the relationship between them, wered able to visualize these chemical agents with a finite mathematical-fluid method and method and by changing the physical parameters of materials. Reagents, reactions, and heat transfer changes can reach the highest efficiency. Using the finite element method, obtained two-dimensional and three-dimensional diagrams and contours that depicted the changes in concentration and temperature of the products and the reactant and showed that they also showed significant changes in the opposite direction. The novelty of this paper is the use of different coefficients of material diffusion constants and also considering the concentration and temperature of materials involved in reacting with non-heat sources and with heat source modes. So that showed the concentration and heat transfer rate of substances

involved in chemical reactions in the form of twodimensional and three-dimensional diagrams to their distance from the borders of the vessel. The main challenge in this article is to investigate the changes in the concentrations of substances involved in chemical reactions around the plate, which are calculated in two cases without internal heat energy or internal heat production. Among the achievements of this article, it can be mentioned that during this article, using the FEM calculation method, the concentrations, and temperatures of the reactant and product materials were analyzed, and the result was obtained that a heat source around the plate, heat transfer and concentration distribution is improved. In general, in the present study, the inner plate's surface meshing was done with the finite element method. The meshing and the number of elements were obtained. In the second part, the preliminary results of the present study were compared with a similar article, and in the third part, with diagrams. Moreover, twodimensional and three-dimensional contours have been used to investigate the temperature and concentration of reactants and products as shown in Figure 1.

1. 1. Problem Definition In this paper, using the reaction and diffusion relations, the reaction between 3 chemical species, and the relationship between temperature changes and the rate of chemical reaction, investigate the temperature and concentration of species around a vessel (according to Figure 2). As described three chemical components, A, B, and C, which react and diffuse, and a temperature, which is affected by the reactions.

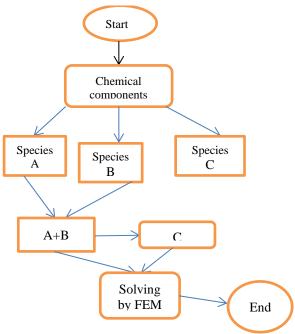


Figure 1. Flowchart of the problem

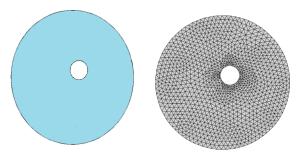


Figure 2. Geometry and mesh of the problem

Assumptions:

- I) A combines with B to form C, liberating heat.
- II) C decomposes to A and B, absorbing heat. The decomposition rate is temperature dependent.
- III) A, B, C and Temperature diffuse with differing diffusion constants.

The boundary of the vessel is held cold, and heat is applied to a circular exclusion patch near the center, intended to model an immersion heater. What is an immersion heater? The simple answer is that it may be a device that gives hot water to your house and is fueled by electricity. The immersion water heater is partitioned from your central warming boiler or radiators, which means that even if your central warming fails, you should still be able to have warm water in your house. A, B, and C cannot diffuse out of the boundary. This example shows the application of FlexPDE to the solution of reaction-diffusion problems. The complete equations, including the Arrhenius terms that describe the system, are [11]:

div
$$(K_1 \cdot \frac{\partial T}{\partial x} \vec{i} + \frac{\partial T}{\partial y} \vec{j} + \frac{\partial T}{\partial z} \vec{k}) + Q + K_1 \cdot e^{-(H_1/(T+273))}$$
. (0.0025).A.B- K₂.e (-H₂/(T+273)). (0.0025).C. (T+273)

div
$$(K_a. \frac{\partial A}{\partial x}\vec{t} + \frac{\partial A}{\partial y}\vec{j} + \frac{\partial A}{\partial z}\vec{k}) - K_1.e^{-(-H_1/(T+273))}.A.B+$$
 (2)
 $K_2.e^{-(-H_2/(T+273))}.C.(T+273) = 0$

div
$$(K_b. \frac{\partial B}{\partial x}\vec{t} + \frac{\partial B}{\partial y}\vec{f} + \frac{\partial B}{\partial z}\vec{k})$$
 - $K_1.e^{(-H_1/(T+273))}$.A.B+ $K_2.e^{(-H_2/(T+273))}$.C. $(T+273) = 0$

div
$$(K_c. \frac{\partial c}{\partial x}\vec{i} + \frac{\partial c}{\partial y}\vec{j} + \frac{\partial c}{\partial z}\vec{k}) + K_1.e^{-(-H_1/(T+273))}.A.B K_2.e^{-(H_2/(T+273))}.C.(T+273) = 0$$
 (4)

where Kt, Ka, Kb, and Kc are the diffusion constants, EABS is the heat liberated when A and B combine, and Q is any internal heat source. A, B, and C are the chemical components, T is the temperature parameter, and H1 and H2 are the activation energy parameter for A+B and C species. K1 is the reaction coefficient for A+B, and K2 is the reaction coefficient for C.

The boundary layer is [11]: in the $(0,-1) \rightarrow \text{Temp}=0$,

$$a^{'}=0,b^{'}=0,c^{'}=0$$
 (5)

In the $(-0.2, 0) \to \text{Temp}=100$,

$$a^{'}=0,b^{'}=0,c^{'}=0$$
 (6)

Notice that the system is non-linear, as it contains terms involving A.B and C.Temp.

There are infinite solutions to these equations, differing only in the total species count. Since species are conserved, the initial conditions uniquely determine the final solution. However, this fact is not embodied in the steady-state equations. The only way to impose this condition on the steady-state system is through an integral constraint equation, which describes the conservation of the total species number.

3. METHODOLOGY

3. 1. Finite Element Method (FEM) A finite element method (abbreviated as FEM) is a numerical method to obtain a surmised solution to a course of problems administered by elliptic partial differential equations. These problems are called boundary value problems, comprising a partial differential equation. (FEM) is an amazingly valuable device within the field of gracious building for numerically approximating physical structures as complex as standard expository arrangements. The advantages of using this method are high adaptability, great accuracy, time-dependent simulation, and better visualization of the boundaries of the studied shape. Similar results can be achieved with other mathematical methods, such as VIM, but they do not have the application of this method. The finite element method can be a fundamental numerical technique. One of the common sense applications for this strategy is the FlexPDE scheme, which realizes the nonlinear fragmentary differential equations and the modulus differential equations. FlexPDE yield is added to a "problem-solving environment" in which the overall strengthening of the valences is working, which is necessary to determine the movable differentiation equation systems.

3. 2. Validation for Methods In this section, for validation, compared our work by Ebermann et al. [11] in Table 1. The amount of computational error in our work is very low compared to Ebermann work. The maximum number of errors happened in x=0.5 and minimum number of errors happened in x=1.

4. RESULTS AND DISCUSSION

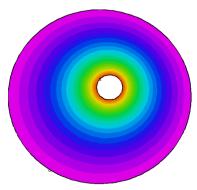
The set of shapes above (Figure 3) shows the temperature changes of reactive particles around the vessel in different heat and heat reaction modes. As mentioned before, around the inner circular vessel and its center, due

to the addition of the heat flow of the boundary layer with high thermal thickness, the thermal flux is maximum in its boundary layer points. As far from the center of the vessel, the crushing vessel is largely spread around, and the temperature of the reaction of the species decreases, and more heat is released, resulting in a small thermal boundary layer. Figures 3(a) and 3(b) show that do not have heat production in the center of the vessel, but due to the import of heat following shapes C-3 and D-3, there is much heat around the inner vessel and hot vortex behind the vessel (a) vessel is formed. In general, with the increase in the heat given to the reactive species (a) and (b), more energy from these species spreads into the environment, a larger boundary layer is formed, and the heat transfer level becomes larger, resulting in increased efficiency and heat flux. The temperature gradient (difference between two arbitrary particles on the plane) of material a has lower values with increasing heat transfer to the center than in the case without a heat source

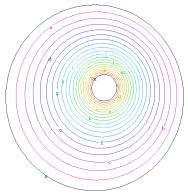
First, describe the relationship between the concentration of reactants and temperature and the thermal diffusion coefficient (according to Figure 4). In general, higher-concentration molecules move to a lower-concentration region, which means that the heat diffusion flux is related

TABLE 1. Comparison of temperature for present work and Ebermann's work [11] at K_t =0.05, H_1 =10, K_1 =1

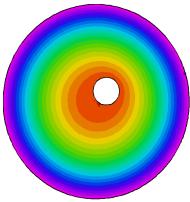
		x = -1.5		x = 0	x = 0.5	x = 0.75	x = 1
Tomn	Present work	0	26	48	68.9	80	10
Temp	Ebermann et al. [11]	0	25.8	49	66.9	80	10
Concentrat	Present work	7.79	7.88	7	8.04	8.34	8
ion	Ebermann et al. [11]	7.79	7.88	7	8.03	8.34	8



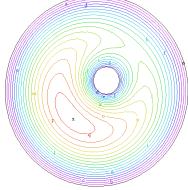
(a) Temperature profile around the vessel for heat source=0



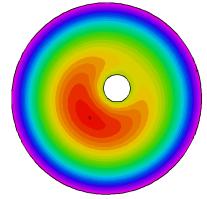
(b) Stream line of temperature profile around the vessl for heat source=0



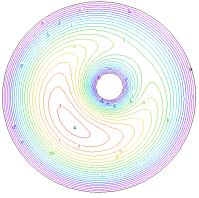
(c) Temperature profile around the vessel for heat source=2



(d) Stream line of Temperature profile for heat source=2



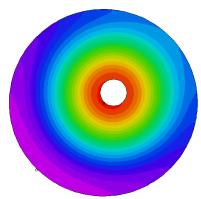
(e) Temperature profile around the vessel for heat source=4



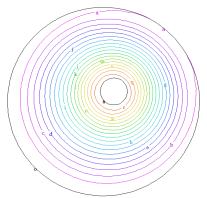
(f) Stream line of Temperature profile for heat source=4

Figure 3. Temperature alterations around the vessel for different values of heat source

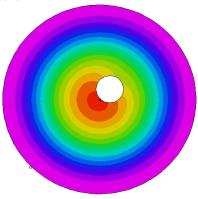
to the concentration gradient. Let us now examine the relationship between the concentration of reactants and temperature. Since the rate of collision of species with each other increases with increasing temperature, concluded that the rate of the chemical reaction is directly related to temperature. Also, the reaction rate increases with increasing reactant concentration and decreases with decreasing concentration. According to Figure 4, reactant concentration (component a) is directly related to temperature and heat transfer, so it increases with increasing temperature concentration and decreases with decreasing temperature. In the case of no heat source, the material concentration is evenly distributed around the inner vessel. Since it is directly related to temperature, the amount of concentration is greater around the circular boundary. As it moves away from the center, this value decreases. By adding a heat source and giving extra heat to the center, reciprocating currents are created with multiple amplitudes. The higher this amount of inlet heat, the larger the reciprocating currents behind the inner vessel. We conclude that the weak flow behind the body increases, and the pressure decreases with increasing heat.



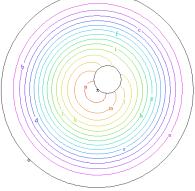
(a) Concentration profile around the vessel for heat source=0



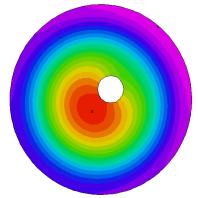
(b) Stream line of concentration profile around the vessel for heat source=0



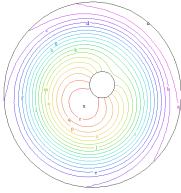
(c) Concentration profile around the vessel for heat source=2



(d) Stream line of concentration profile around the vessel for heat source=2



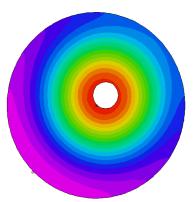
(e) Concentration profile around the vessel for heat source=4



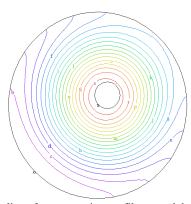
(f) Stream line of concentration profile around the vessel for heat source=4

Figure 4. Concentration alterations around the vessel for different values of heat source for component (a)

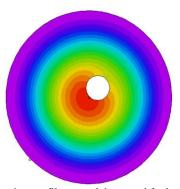
Figure 5 shows the changes in the concentration of reactant (b) around the plate and that the species is scattered around with a high diffusion coefficient. The higher the heat given to the center of the plate, the higher the specie diffusion coefficient and the better the reaction rate for the formation of substance (c).



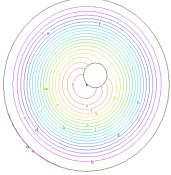
(a) Concentration profile around the vessel for heat source=0 for component (b)



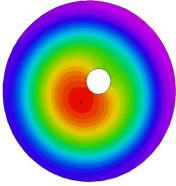
(b) Stream line of concentration profile around the vessel for heat source=0 for component (b)



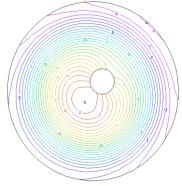
(c) Concentration profile around the vessel for heat source=2 for component (b)



(d) Stream line of concentration profile around the vessel for heat source=2 for component (b)

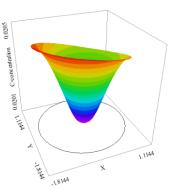


(e) Concentration profile around the vessel for heat source=2 for component (b)

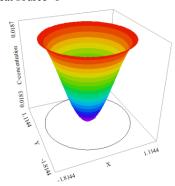


(f) Stream line of concentration profile around the vessel for heat source=2 for component (b)

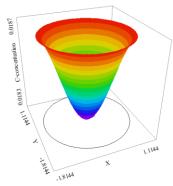
Figure 5. Concentration alterations around the vessel for different values of heat source for component (b)



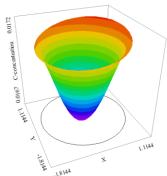
(a) 3D concentration profile for component (c) near the vessel by heat source=0 $\,$



(b) 3D concentration profile for component (c) near the vessel by heat source=2 .



(b) 3D concentration profile for component (c) near the vessel by heat source=2

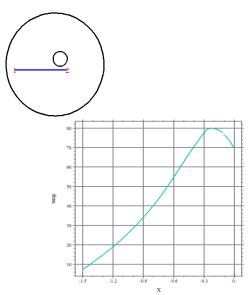


(c) 3D concentration profile for component (c) near the vessel by heat source=4

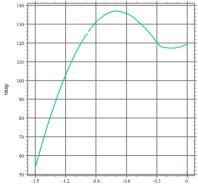
Figure 6. Three-dimensional images concentration alterations around the vessel for component (c)

The above figures (Figure 6) show in 3D the concentration of exothermal c around the vessel. In contrast to the previous states of species (a) and (b), where heat is dissipated from the center around, in this case, the heat around the center is greater. This is because substance (c) releases heat during a reaction and breaks it down into species a and b. Due to the addition of a heat source, the higher the heat and temperature around substance (c), the smaller the thermal boundary layer around the inner vessel and the larger around the outer vessel, and the greater the concentration around the boundary layer, the thicker it becomes. As the concentration increases, the viscosity increases, and the speed slows down.

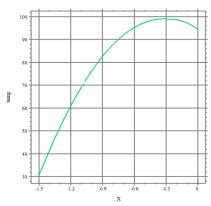
The diagrams in Figure 7 show the temperature composition changes of the materials involved in the chemical reaction at different heat sources at regular intervals. Given these changes on a graph and the



(a) Two dimensional graph of temperature changes in terms of distance from the center of the vessel to outside the environment for heat source=0



(b) Two dimensional graph of temperature changes in terms of distance from the center of the vessel to outside the environment for Heat source=4



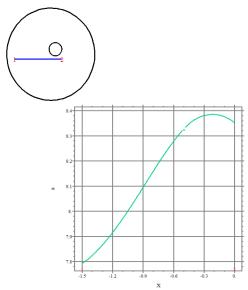
(c) Two dimensional graph of temperature changes in terms of distance from the center of the vessel to outside the environment for Heat source =2

Figure 7. Temperature changes of reacting materials at certain intervals with different heat sources

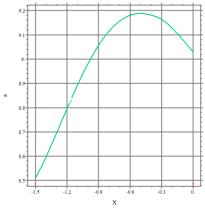
numerical representation of each distance, interpret the results with a very low error rate. In the case without a heat source and low diffusion coefficient, according to Figure 7(a), with increasing distance from x = -1.5 to x =0, the graph ascends, and the temperature increases to reach the peak. At x = -0.2, have the maximum temperature, which is the thermal peak. The temperature at this point is 80 degrees. Now, by adding a heat source in Figures 7(b) and 7(c), these graphical changes are created with larger amplitude, and a more extensive thermal boundary layer is formed around the central vessel. On average, temperature changes and heat transfer in the distance from the center to the surroundings in the maximum heat source mode is about 65% more than the average heat source mode and about 44% more than the non-heat source mode.

Figure 8 shows the diagrams of changes in the diffused concentration of reactant around the skeletal boundaries of the vessel with different heat sources. According to Figure 8(a), the closer get to the center of the vessel shape, the higher the concentration of the reaction material, increasing viscosity. This description applies to other diagrams as well and applies to them as well. Adding a heat source to the center around the vessel shape increases the concentration of the reactants, thus increasing the heat released from them. The lower the heat transfer to the center, the less heat is released and the lower the concentration. The maximum value of concentration occurs at x=-0.6 in the heat source=4. On average, concentration changes in the distance from the center to the surroundings in the maximum heat source mode is about 57% more than the average heat source mode and about 28% more than the non-heat source

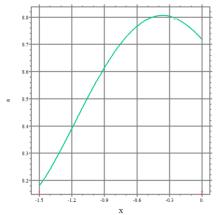
Table 2 shows the diagrams of changes in the diffused concentration of reactant around the skeletal boundaries of the vessel with different heat sources. According to



(a) Two dimensional graph of concentration component (a) changes in terms of distance from the center of the vessel to outside the environment for heat source=0



(b) Two dimensional graph concentration component (a) in terms of distance from the center of the vessel to outside the environment for source=4



(c) Two dimensional graph of concentration component (a) in terms of distance from the center of the vessel to outside the environment for Heat source =2

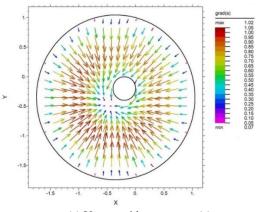
Figure 8. Concentration changes of reacting materials at certain intervals with different heat sources

TABLE 2. Numerical comparison of concentration between different heat sources for component (c)

X	Heat source=0	Heat source=2	Heat source=4	
-1.5	2.04	1.87	1.71	
-1.4	2.02	1.82	1.65	
-1.3	2.01	1.71	1.58	
-1	1.88	1.44	1.22	
-0.6	1.56	0.89	1	
-0.2	1.09	0.76	0.83	
0	1	0.54	0.60	

Table 2, the maximum amount of concentration exists at x=-1.5 for heat source=0 and the minimum concentration exists at x=0 for heat source=4 by C=0.60. According to the numbers obtained in the table above, concluded that as the intensity of heat transfer to the center of the vessel increases, the concentration of reactant material (c) decreases, and the lower the temperature, the higher the concentration. On average, concentration changes in the distance from the center to the surroundings in the maximum heat source mode is about 76% less than the average heat source mode and about 14% less than the non-heat source mode. By releasing heat, substance c decomposes into materials (a) and (b) and emits some heat. This indicates that as the diffusion coefficient of the decomposed material increases, the concentration of the material decreases, and the reaction rate increases.

As seen in the above images (Figure 9), the movement vector of the material particles involved in the chemical reactions around the vessel and the temperature gradient lines of the reacting and produced particles have been drawn. The temperature vector lines for reacting particles (a) and (b) around the inner vessel have low values; because heat is released and their size is small. However, passing through the internal boundary layer makes this vector larger than the initial state. Particle (c)



(a) Vector grid component (a)

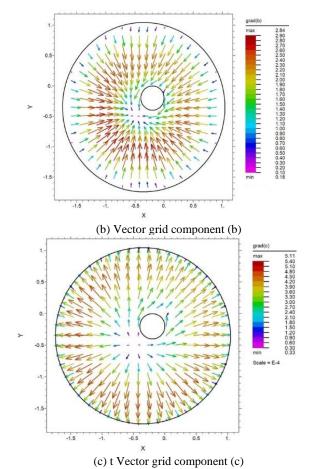


Figure 9. Simulation of motion vector of chemical reaction particles for temperature parameter

absorbs heat because it decays. This article's thermal lines around the outer vessel's boundaries have larger sizes than the lines near the boundaries of the inner vessel.

4. CONCLUSION

In this paper, investigated the temperature and concentration of species around a vessel using the reaction and diffusion relations and the reaction between 3 chemical species, and the relationship between temperature changes and the rate of a chemical reaction. The novelty of this paper is the use of different coefficients of material diffusion constants and also considering the concentration and temperature of materials involved in reacting with non-heat sources and with heat source modes so that based on heat sources with different degrees of temperature and showed the concentration of reactant and product in the form of graphs and contours by FEM method. The finite Element Method is utilized for calculated differential equations.

- According to the results obtained, when the temperature of the reactants increases and more heat is released, the concentration also changes a lot, and its amount increases, but in products such as substance c, it has an inverse relationship with reactants a and b in such a way that As the concentration and temperature of the reactants increase, these values decrease in the product.
- Temperature changes and heat transfer in the distance from the center to the surroundings in the maximum heat source mode is about 65% more than the average heat source mode and about 44% more than the non-heat source mode.
- On average, concentration changes in the distance from the center to the surroundings in the maximum heat source mode is about 57% more than the average heat source mode and about 28% more than the non-heat source mode.

5. REFERENCES

- Waqas, M., "Simulation of revised nanofluid model in the stagnation region of cross fluid by expanding-contracting cylinder", *International Journal of Numerical Methods for Heat* & Fluid Flow, (2019). doi: 10.1108/HFF-12-2018-0797.
- Farooq, S., Khan, M.I., Waqas, M., Hayat, T. and Alsaedi, A., "Transport of hybrid type nanomaterials in peristaltic activity of viscous fluid considering nonlinear radiation, entropy optimization and slip effects", *Computer Methods and Programs* in *Biomedicine*, Vol. 184, (2020), 105086. doi: 10.1016/j.cmpb.2019.105086.
- Waqas, M., "A mathematical and computational framework for heat transfer analysis of ferromagnetic non-newtonian liquid subjected to heterogeneous and homogeneous reactions", *Journal* of *Magnetism and Magnetic Materials*, Vol. 493, (2020), 165646. doi: 10.1016/j.jmmm.2019.165646.
- Waqas, M., "Chemical reaction impact in dual diffusive nonnewtonian liquid featuring variable fluid thermo-solutal attributes", *Chemical Physics Letters*, (2022), 139661. doi: 10.1016/j.cplett.2022.139661.
- Waqas, M., Nisar, U., Shehzad, S., Irfan, M. and Khan, W., "A non-linear mathematical analysis of thermally radiative stratified nanoliquid featuring the aspects of magnetic field, robin conditions and thermal radiation", *International Communications in Heat and Mass Transfer*, Vol. 125, (2021), 105199. doi: 10.1016/j.icheatmasstransfer.2021.105199.
- Waqas, M., "Diffusion of stratification based chemically reactive jeffrey liquid featuring mixed convection", *Surfaces and Interfaces*, Vol. 23, (2021), 100783. doi: 10.1016/j.surfin.2020.100783.
- Waqas, M., Hayat, T., Alsaedi, A. and Khan, W.A., "Analytical evaluation of oldroyd-b nanoliquid under thermo-solutal robin conditions and stratifications", *Computer Methods and Programs in Biomedicine*, Vol. 196, (2020), 105474. doi: 10.1016/j.cmpb.2020.105474.
- Waqas, M., Sadiq, M.A. and Bahaidarah, H.M., "Gyrotactic bioconvection stratified flow of magnetized micropolar nanoliquid configured by stretchable radiating surface with joule heating and viscous dissipation", *International Communications* in *Heat and Mass Transfer*, Vol. 138, (2022), 106229. doi: 10.1016/j.icheatmasstransfer,2022.106229.

- Guedri, K., Khan, W., Alshehri, N.A., Mamat, M., Jameel, M., Xu, Y.-J., Waqas, M. and Galal, A.M., "Thermal aspects of magnetically driven micro-rotational nanofluid configured by exponential radiating surface", *Case Studies in Thermal Engineering*, Vol. 39, (2022), 102322. doi: 10.1016/j.csite.2022.102322.
- Waqas, M., Alzahrani, F. and Khan, M.I., "Transport of chemically reactive thixotropic nanofluid flow by convectively heated porous surface", *Chemical Physics Letters*, Vol. 803, (2022), 139742. doi: 10.1016/j.cplett.2022.139742.
- Ebermann, M., Bogenfeld, R., Kreikemeier, J. and Glüge, R., "Analytical and numerical approach to determine effective diffusion coefficients for composite pressure vessels", *Composite Structures*, Vol. 291, (2022), 115616. doi: 10.1016/j.compstruct.2022.115616.
- Shadman, P., Parhizi, Z., Fathollahi, R., Zarinfar, M., Anisimova, E.Y. and Pasha, P., "Combined septum and chamfer fins on threated stretching surface under the influence of nanofluid and the magnetic parameters for rotary seals in computer hardware", *Alexandria Engineering Journal*, Vol. 62, (2023), 489-507. doi: 10.1016/j.aej.2022.07.044.
- Fathollahi, R., Hesaraki, S., Bostani, A., Shahriyari, E., Shafiee, H., Pasha, P., Chari, F.N. and Ganji, D.D., "Applying numerical and computational methods to investigate the changes in the fluid parameters of the fluid passing over fins of different shapes with the finite element method", *International Journal of Thermofluids*, Vol. 15, (2022), 100187. doi: 10.1016/j.ijft.2022.100187.
- 14. Abdollahzadeh, M.J., Fathollahi, R., Pasha, P., Mahmoudi, M., Samimi Behbahan, A. and Domiri Ganji, D., "Surveying the hybrid of radiation and magnetic parameters on maxwell liquid with TiO₂ nanotube influence of different blades", *Heat Transfer*, Vol. 51, No. 6, (2022), 4858-4881. doi: 10.1002/htj.22526.
- Pasha, P. and Domiri-Ganji, D., "Hybrid analysis of micropolar ethylene-glycol nanofluid on stretching surface mounted

- triangular, rectangular and chamfer fins by fem strategy and optimization with RSM method", *International Journal of Engineering, Transactions B: Applications*, Vol. 35, No. 5, (2022), 845-854. doi: 10.5829/IJE.2022.35.05B.01.
- Darezereshki, E., Behrad Vakylabad, A. and Yousefi, M., "Chemical process of synthesizing zinc oxide (ZnO) with nanorod and spherical morphologies", *International Journal of Engineering, Transactions B: Applications*, Vol. 34, No. 8, (2021), 1888-1897. doi: 10.5829/ije.2021.34.08b.10.
- Wang, B., Wang, Z., Sun, C. and Wu, Y., "Numerical investigation of the heat-fluid characteristic inside high-speed angular contact ball bearing lubricated with grease", *International Journal of Engineering, Transactions B: Applications*, Vol. 34, No. 5, (2021), 1313-1320. doi: 10.5829/ije.2021.34.05b.26.
- Madani, M., Lin, K. and Tarakanova, A., "Dsressol: A sequence-based solubility predictor created with dilated squeeze excitation residual networks", *International Journal of Molecular Sciences*, Vol. 22, No. 24, (2021), 13555. doi: 10.3390/ijms222413555.
- Kunkel, G., Madani, M., White, S.J., Verardi, P.H. and Tarakanova, A., "Modeling coronavirus spike protein dynamics: Implications for immunogenicity and immune escape", *Biophysical Journal*, Vol. 120, No. 24, (2021), 5592-5618. doi: 10.1101/2021.08.19.456973.
- Hosseini, S., Roostaei, M., Mosavi Mashhadi, M. and Faraji, G., "Fabrication of al/mg bimetallic thin-walled ultrafine-grained tube by severe plastic deformation", *Journal of Materials Engineering and Performance*, Vol. 31, No. 5, (2022), 4098-4107. doi: 10.1007/s11665-021-06514-5.
- Alrwashdeh, S.S., Ala'a, M. and Murtadha, T.K., "Effect of turbocharger compression ratio on performance of the sparkignition internal combustion engine", *Emerging Science Journal*, Vol. 6, No. 3, (2022), 482-492. doi: 10.28991/ESJ-2022-06-03-04

Persian Abstract

جكىدە

در این مقاله دما و غلظت گونه ها در اطراف یک ظرف با استفاده از روابط واکنش و انتشار، واکنش بین ۳ گونه شیمیایی و رابطه بین تغییرات دما و سرعت یک واکنش شیمیایی بررسی شده است. نکته جدید این مقاله استفاده از ضرایب مختلف ثابت های انتشار مواد و همچنین در نظر گرفتن غلظت و دمای مواد در گیر در واکنش با منابع غیرحرارتی و با حالت های منبع گرمایی است به طوری که غلظت و سرعت انتقال حرارت مواد در گیر را نشان می دهد. واکنش های شیمیایی به شکل نمودارهای دو بعدی و سه بعدی در مورد فاصله آنها از مرزهای ظرف. با توجه به نتایج بهدست آمده، زمانی که دمای واکنش دهنده ها افزایش می یابد و گرمای بیشتری آزاد می شود، غلظت نیز تغییر زیادی کرده و مقدار آن افزایش می یابد. اما در محصولاتی مانند ماده (ج) با واکنش دهنده های (الف) و (ب) رابطه معکوس دارد به گونه ای که با افزایش غلظت و دمای واکنش دهنده ها، این مقادیر در محصول کاهش می یابد. به طور متوسط، تغییرات غلظت در فاصله از مرکز تا محیط اطراف در حالت منبع حرارت حداکثر حدود ۷۲ درصد کمتر از حالت منبع حرارت غیر گرما است.