



Using the Genetic Algorithm Based on the Riedel Equation to Predict the Vapor Pressure of Organic Compounds

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ABSTRACT

In this paper, a genetic algorithm (GA) has been used to predict the vapor pressure of pure organic compounds based on Riedel equation. Initially, the coefficients of Riedel equation were optimized. Then, a new term was added to the original Riedel equation to reduce error of the model in prediction of vapor pressures of pure materials. 110 components at two different pressures (10 and 100 kPa) were chosen to investigate the capability of mentioned models. Absolute average relative deviation percent (AARD %) was reported for 40 components as testing materials to compare the calculated results of two models with experimental data. Results showed that the exerted modification on Riedel equation decreases the errors in prediction of vapor pressures of chemical components.

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1. INTRODUCTION

Vapor pressure equation represents the relationship between the vapor pressure of a liquid and temperature. When the vapor phase is in equilibrium with the liquid phase. Clapeyron equation can be obtained from the equality of chemical potential, temperature and pressure in both phases [1]. The first equation for prediction of the vapor pressure of pure compounds was presented by integration of Clapeyron equation. Later many equations were suggested by modifying the original equation. Most of these equations are based on the principle of corresponding states and usually are presented as the logarithm of the reduced vapor pressure versus the reduced temperature. Antoine offered a modified simple form of the vapor pressure equation, in 1888 [2]. Cox presented a linear graph that relates the logarithm of the vapor pressure and temperature of few materials. Later this correction was extended for more compounds [3]. Wagner offered an equation to calculate the vapor pressure of nitrogen and argon, over the entire temperature range which the experimental data of vapor

pressure were available [4]. Moreover, a new form of Wagner's equation was proposed by Ambrose and Giassee which could successfully be applied for vapor pressure prediction of most compounds [5]. But one of the most important equations which is widely used for prediction of vapor pressure is Riddle equation [6, 7]. It is a predictive expression for calculation of vapor pressures of various components which involves some coefficients. The coefficients of Riedel equation are reported in literatures for different compounds [8, 9]. But to improve the capability of this equation, it is possible to optimize its coefficient. Olsen et al. [10] presented a model for vapor pressure prediction of the volatile organic compounds (VOCs) at 20 °C from their chemical (UNIFAC) structure. Velasco et al. [11] proposed a simple equation for vapor pressure estimation of pure compounds from their triple points to the critical points. The suggested equation was tested for 53 pure compounds by applying NIST program. The vapor pressure data of these substances obtained from proposed equation with an overall average deviation of 0.55% [11]. Gandhidasan et al. [12] predicted vapor pressures of aqueous desiccants for cooling applications using an ANN model. Rohani et al. [13] correlated the

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liquid density and the vapor pressure of 20 pure alcohols using an ANN model and statistical associating fluid theory (SAFT) equation of state. They reported the average absolute deviation percent (ADD%) for vapor pressure of pure alcohols for SAFT equation of state and ANN model were 3.378 and 3.593%, respectively [13]. Honarmand et al. [14] presented an accurate artificial neural network (ANN) model for vapor pressures prediction of pure substances. They used more than 12000 vapor pressure data point for testing, training and validation of ANN model. They reported that the ANN model predicted the vapor pressure of 75 pure compounds with average absolute relative deviation of 0.211% [14]. Roganov et al. [15] developed an algorithm based on a set of saturated vapor pressures of substances at various temperatures for calculation of the critical pressures, the critical temperatures, and Riedel coefficients at a critical point. Hogge et al. [16] optimized the final coefficient of Riedel equation (denoted as E) for vapor pressure estimation of seven various families of compounds including n-alkanes, 2-methyl alkanes, 1-alkenes, n-aldehydes, aromatics, ethers and ketones. They found out that the E equal 2 fits these compounds much better than the common E of 6 [16]. Also, they reported that an E of 2-5 fits compounds such as aldehydes, alkanes, alkenes, alkynes, amines, aromatics, esters, ethers, gases, halogenated compounds, ketones, multifunctional compounds, ringed alkanes, silanes, and sulfides much better than the usual E of 6 [17]. Since, GA is a new powerful tool for optimization it can be used to perform modification of Riedel equation.

In this article the Riedel's coefficients were optimized using vapor pressure data of 110 components at two different pressures (10 and 100 kPa) by applying GA. Also, a new equation based on Riedel equation was proposed for estimation of the vapor pressure, specially at low pressure.

2. THEORY

Riedel presented the following equation to calculate the vapor pressure of various compounds:

$$\ln P_{vp} = A + \frac{B}{T} + C \ln T + D T^6 \quad (1)$$

where, P_{vp} and T are the vapor pressure and the temperature, respectively. Parameters A , B , C , and D , are constants that are function of temperature, critical temperature (T_c), normal boiling temperature (T_b), and critical pressure (P_c). Riedel has defined the parameter α to determine the constants of Equation (1):

$$\alpha = \frac{d \ln P_{vpr}}{d \ln T_r} \quad (2)$$

Where P_{vpr} and T_r are reduced vapor pressure and reduced temperature which are equal to P/P_c and T/T_c , respectively.

Respect to available experimental data for vapor pressure, Riedel and Plank have shown that:

$$\frac{d\alpha}{dT_r} = 0 \quad \text{At} \quad T_r = 1 \quad (3)$$

According to Equation (3) Riddle has suggested the following equations:

$$\ln P_{vpr} = A^+ - \frac{B^+}{T_r} + C^+ \ln T_r + D^+ T_r^6 \quad (4)$$

$$A^+ = -35Q \quad B^+ = -36Q$$

$$C^+ = 42Q + \alpha_c \quad D^+ = -Q \quad (5)$$

Riedel correlated the experimental vapor pressure data of different pure substances and suggested Equation (6) for estimation of empirical parameter Q as follow:

$$Q = K(3.758 - \alpha_c) \quad (6)$$

α_c is the parameter α at critical point and could be obtained by the following equations:

$$\alpha_c = \frac{3.758K\psi_b + \ln(P_c/1.01325)}{K\psi_b - \ln T_{br}} \quad (7)$$

$$\psi_b = -35 + \frac{36}{T_{br}} + 42 \ln T_{br} - T_{br}^6 \quad (8)$$

Where T_{br} is the reduced normal boiling temperature which equals to T_b/T_c . Also, Riddle considered the value of K for all compounds, equal to 0.0838. Later, Vetere [8] showed that for calculation of K , more accurate results will be achieved using the following equations for alcohols and acids:

$$\text{For Acids: } K = 0.12 + 0.025h \quad (9)$$

$$\text{For Alcohols : } K = 0.373 - 0.03h \quad (10)$$

$$h = T_{br} \frac{\ln(P_c/1.01325)}{1 - T_{br}} \quad (11)$$

Riddle equation was obtained by the integration of Clapeyron equation, assuming the linearity of the enthalpy changes with temperature. This equation can predict with high accuracy, the vapor pressure of pure compounds using the initial data including T_b , T_c and P_c [8]. But there is a problem in using this equation and it is the lack of high accuracy for prediction of the vapor pressure for compounds at low pressures. Vetere expressed that the most important defect of the model, is the failure of equation to predict the behavior of the vapor pressure of compounds at low temperatures [9]. Some researchers have suggested the extrapolation of the experimental data for vapor pressures at low pressures [18, 19]. Also, the measurement of heat capacity at low temperatures and applying it in the Clapeyron equation can be used [20-22]. The

extrapolation of the results of vapor pressure equations at low temperatures is one of the theoretical methods to predict the vapor pressure of compounds at low pressures [9, 23]. Another solution for calculation of the vapor pressure is modification of the main Riedel equation. In this work, initially, 10 fixed parameters in the Riedel equation have been optimized using the genetic algorithm. The modified equation has been used to obtain the temperature at which the vapor pressure of studied component reaches to 10 and 100 kPa. Main equations that should be optimized are:

$$\Psi_b = -C_1 + \frac{C_2}{T_{br}} + C_3 \ln T_{br} - T_{br}^{C_4} \quad (12)$$

$$\alpha_c = \frac{C_5 \Psi_b + \ln(P_c/1.01325)}{K \Psi_b - \ln T_{br}} \quad (13)$$

$$Q = K(C_6 - \alpha_c) \quad (14)$$

$$A^+ = -C_9 Q \quad B^+ = -C_8 Q \quad (15)$$

$$C^+ = C_7 Q + \alpha_c \quad D^+ = -Q$$

$$\ln P_{vpr} = A^+ - \frac{B^+}{T_r} + C^+ \ln T_r + D^+ T_r^{C_{10}} \quad (16)$$

Where, C_1 to C_{10} are the coefficients, which should be optimized. Moreover, a new equation was proposed for achieving to a greater accuracy by adding a new term to the Riedel equation:

$$\ln P_{vpr} = A^+ - \frac{B^+}{T_r} + C^+ \ln T_r + D^+ T_r^{C_{10}} - C_{11} T_r \quad (17)$$

In this case, 11 parameters (C_1 to C_{11}) of Equation (17) were calculated by applying the genetic algorithm.

2. 1. Genetic Algorithm Genetic algorithm (GA) uses the natural evolution and survival of the fittest method with the genetic reproduction for quick search and optimization. The most important aspect of (GA) is that, it can do the search to find the best among the possible answers in the interval that was chosen by the user. It can find the optimal answer after several iterative calculations, according to the survival of the fittest law. Search process consists of artificial mutation, crossover and selection operations [24-27]. Figure 1 shows the steps of genetic algorithm for optimization of coefficients of Equations (12) and (17). Steps of operations can be described as follows:

1. First, $C_1, C_2, C_3 \dots C_{10}$ for Equations (12-16) and $C_1, C_2, C_3 \dots C_{11}$ for Equations (12-15) and (17) were coded to form the chromosomes. The chromosome X is expressed in the form of $X = \{k1, k2 \dots k10\}$ for Equations (12-16) and in form of $X = \{k1, k2 \dots k11\}$

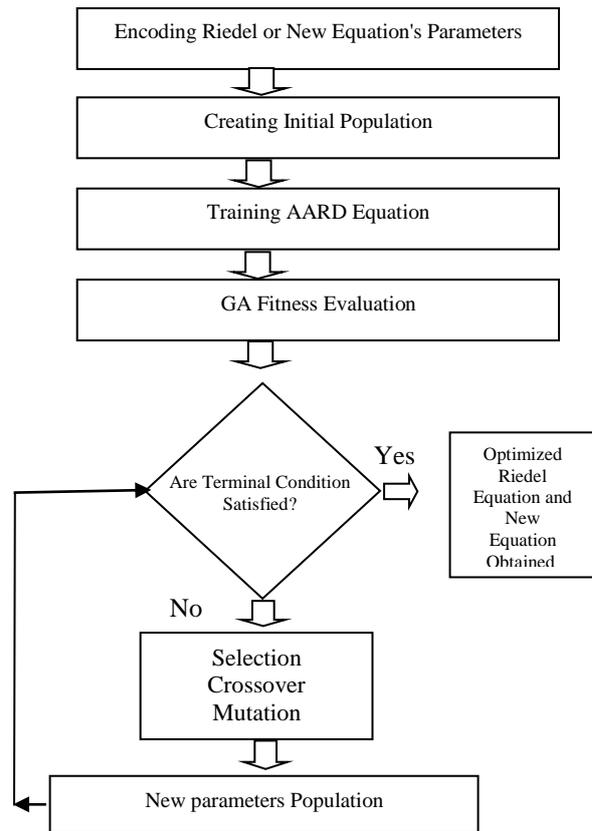


Figure 1. Steps of genetic algorithm to optimize the coefficients of Riedel and new suggested equation

for Equations (12-15) and (17) in which $k1, k2 \dots k11$ are the same coefficients as $C_1, C_2, C_3 \dots C_{11}$. The population size and the maximum evolution for generations were considered 50 and 100, respectively. The start of generations was from zero.

2. Evaluation function: In this step, the absolute average relative deviation percent (AARD %) for vapor pressures data was considered as the evaluation function:

$$AARD\% = \frac{100}{n} \times \sum_{i=1}^n \left| \frac{P^{exp} - P^{cal}}{P^{exp}} \right| \quad (18)$$

Where P^{cal} is calculated vapor pressure by the models and P^{exp} is the experimental value of the vapor pressure for each substance.

3. Choice: the stochastic uniform method was used to decide whether the chromosome must be alive in the next generation or not. The chromosome that stayed alive in the next generation is placed in the Crossover and Mutation operations.

4. Crossover: The intersection occurs between the parents to form a new child with the intersection ability. The possibility of generation for new chromosome in each pair was considered equal to 0.8 and the scattered

function was used for newly constructed chromosomes to make up the next generation.

5. Mutation: The Mutation operation follows the Crossover operation and determines whether a chromosome should be changed in the next generation or not. In this step, Gaussian method and Scale and Shrink was set equal to one.

6. The next generation: prepares a population for the next generation.

7. Stop conditions: The mentioned operations will be repeated until the number of generations reach to 50.

3. RESULTS AND DISCUSSION

It is important to explain that in this work, two general models based on Riedel equation using the genetic algorithm, have been used to estimate the vapor pressure of organic compounds at pressures of 10 and 100 kPa. At first, efforts have been done to optimize the coefficients of the Riedel equation using the genetic algorithm. In the second model, the coefficients of a new proposed equation have been optimized by changing the main Riedel equation. Finally, the results

of new model have been compared with the first model and also the optimized Riedel equation. During the survey in this work, the vapor pressure data of 150 different organic compounds were applied for pressures of 10 and 100 kPa. 110 data were used in the training phase to obtain the coefficients of the optimized Riedel equation and the coefficients of the new equation. Then, vapour pressures data of 40 different organic compounds were obtained for testing and comparison phase of three equations: The Riedel, the optimized Riedel and the new equation. The list and properties of some used compounds in the training and testing phases are summarized in Tables 1 and 2, respectively [28]. Complete set of data will be available as "Supplemental file" for readers. The optimized coefficients of the Riedel equation by the genetic algorithm method and optimized coefficients of the new equation for pressures of 100 and 10 kPa are listed in Tables 3 and 4, respectively. These coefficients were obtained by minimizing the AARD% introduced in Equation (18). The values of AARD% calculated by applying three mentioned models (Riedel, optimized Riedel and new equation) for vapor pressures of 100 and 10 kPa, are shown in Tables 5 and 6, respectively.

TABLE 1. Characteristics of the used compounds in the training phase [28].

NO.	Mol. form.	Name	T _b (K)	T _c (K)	P _c (bar)	T (°C) at 10 kpa	T (°C) at 100 kpa
1	CBrClF ₂	Bromochlorodifluoromethane	269.2	426.9	42.6	-51.8	-4.3
2	CBrF ₃	Bromotrifluoromethane	215.41	340.15	39.7	-96.6	-58.1
3	CBr ₂ F ₂	Dibromodifluoromethane	295.94	471.3	45.3	-30	22.5
4	CClF ₃	Chlorotrifluoromethane	191.71	301.84	38.73	-116	-81.7
5	CCl ₂ F ₂	Dichlorodifluoromethane	243.45	385.1	41.3	-71.3	-30

TABLE 2. Characteristics of the used compounds in the testing phase [28]

NO.	Mol. form.	Name	T _b (K)	T _c (K)	P _c (bar)	T (°C) at 10 kpa	T (°C) at 100 kpa
1	C ₂ H ₄ Br ₂	1,2-Dibromoethane	404.8	583	71.64	62.2	130.9
2	C ₂ H ₄ O ₂	Acetic acid	391.04	594.45	57.9	55.9	117.5
3	C ₂ H ₅ F	Fluoroethane	235.6	375.31	49.62	-78.7	-37.9
4	C ₄ H ₆	1,3-Butadiene	268.74	425	42.63	-51.9	-4.7
5	C ₄ H ₈	cis-2-Butene	276.8	435.5	41.55	-44.8	3.4

TABLE 3. The coefficients of the optimized Riedel and new equation, for pressure of 100 kPa

Method	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈	C ₉	C ₁₀	C ₁₁
Optimized Riedel	0.152	0.443	0.003	0.633	0.612	0.049	0.867	0.94	0.51	0.625	-
New Equation	0.686	2.548	0.264	1.19	-0.31	0.094	-0.429	2.561	0.592	0.485	0.012

TABLE 4. The coefficients of the optimized Riedel and new equation, for pressure of 10 kPa

Method	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈	C ₉	C ₁₀	C ₁₁
Optimized Riedel	-0.63	1.091	0.41	1.959	3.435	0.695	0.794	0.781	1.046	2.405	-
New Equation	1.345	2.961	0.122	3.468	2.304	1.789	1.154	3.526	1.466	3.433	1.192

TABLE 5. Comparison of errors of Riedel, optimized Riedel and new equation for pressure of 100 kPa

Method	Total absolute percentage error training phase	Total absolute percentage error testing phase	Total absolute percentage error for all substances
Riedel	2.723	3.3555	2.8921
Optimized Riedel	1.8451	3.2389	2.1989
New Equation	1.3840	2.2843	1.6217

TABLE 6. Comparison of errors of Riedel, optimized Riedel and new equation for pressure of 10 kPa

Method	Total absolute percentage error training phase	Total absolute percentage error testing phase	Total absolute percentage error for all substances
Riedel	7.6301	8.3771	7.8293
Optimized Riedel	6.057	7.5838	6.4696
New Equation	3.9060	4.2112	4.0063

As can be seen from the results in Table 5, the average absolute value of the total error decreases by optimizing the Riedel coefficients for prediction of the vapor pressure in both training and testing phases. The errors for pressure of 100 kPa, were reduced from 2.72 to 1.84 percent in training phase and from 3.35 to 3.23 percent in testing phase.

Also, the new suggested equation decreased the average value of the total error to 1.38 and 2.28 percent in the training and testing phase, respectively. But as noted, the fundamental weakness of the Riedel equation is at low pressures and this issue is clearly visible due to the absolute value of the total error for pressure of 10 kPa in the training and testing phase (7.63 and 8.37 percent) and comparing it with the absolute value of the total error for pressure of 100 kPa. According to the results of Table 6 it can be seen that by optimizing the coefficients of the Riedel equation, the training and testing phase errors were reduced to 6.05 and 7.23 percent, respectively. However, a significant decrease of the error was obtained by applying the proposed equation. The training and testing phase errors of

calculations using new model were reduced to 3.90 and 4.21 percent, respectively. Scatter plots of actual versus predicted vapor pressure using optimized Riedel equation and new equation at two pressures (10 and 100 kPa) are shown in Figure 2.

4. CONCLUSION

In this paper, the genetic algorithm was used to optimize Riedel equation. This method is used to calculate the best coefficients of the Riedel and the new suggested model based on Riedel equation for reducing the error of the models in prediction of vapor pressures of chemical components. The advantage of GA is that it can find the optimal coefficients of the equations quickly and with less error. Also with suggestion of a new equation, the optimized results of this equation were compared with the results of both Riedel and the optimized Riedel models. The deviation of Riedel models in the test stage was 3.35 for pressure of 100 kPa. While the optimized Riedel equation showed a deviation of 3.23% for vapor pressure of testing data. The new suggested model deviates from the experimental data for testing phase of GA 2.28%. Due to the weakness of Riedel equation in prediction of low values of the vapor pressure, the optimization done for Riedel equation showed a significant improvement in the result of the model for calculation of vapor pressures. Also, more improvement can be seen using the new suggested model. Comparison of the calculated temperature in which the vapor pressure would be 10 kPa with experimental data showed while the deviation of the main Riedel equation for testing phase of GA was 8.38%; the error of optimized Riedel and new equation for the same data were 7.58% and 4.21%, respectively. By comparison of the obtained errors of studied models it can be concluded that it is possible to achieve more accurate results for the prediction of vapor pressures using the genetic algorithm. Also, it can be seen that the new method has a less error than the Riedel model in prediction of vapor pressure of organic compounds, especially at a low pressure. Beside an increase in accuracy of the model, present study showed that the genetic algorithm addition to high precision has a high speed in optimizing the coefficients of the working equation.

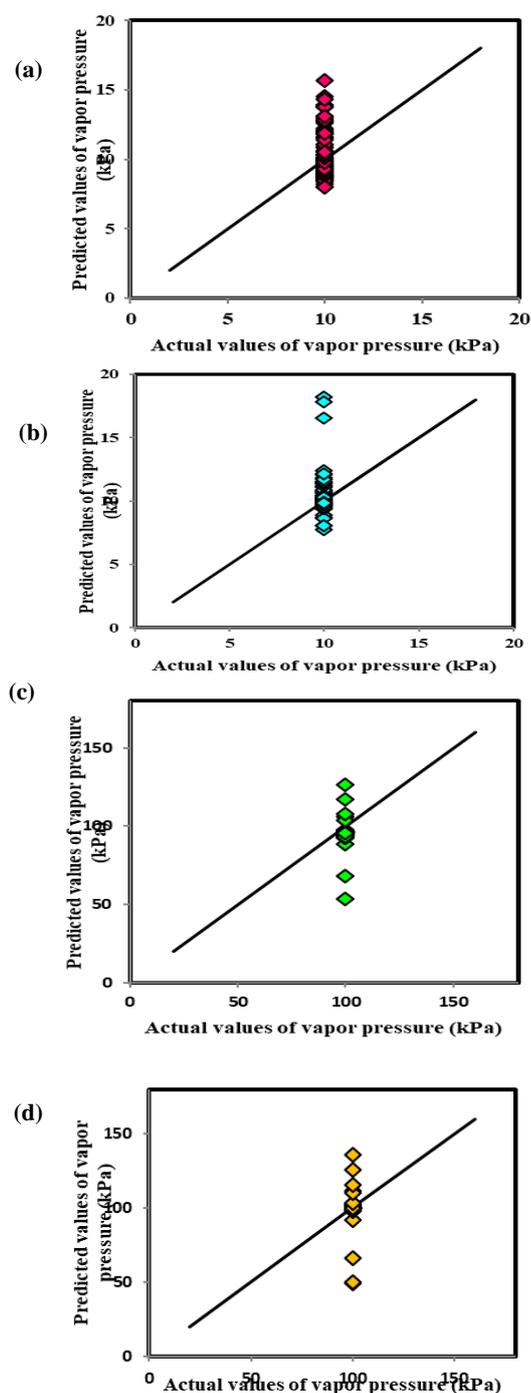


Figure 2. Scatter plots of actual vs. predicted vapor pressure using: (a) optimized Riedel equation at 10 kPa (b) new equation at 10 kPa (c) optimized Riedel equation at 100 kPa (d) new equation at 100 kPa.

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در این مقاله از الگوریتم ژنتیک برای پیش بینی فشار بخار ترکیبات آلی خالص بر پایه معادله ریدل استفاده شده است. در این کار ابتدا با انتخاب 110 ماده مختلف به بهینه سازی ضرایب معادله ریدل برای کاهش خطای ناشی از این روش در پیش بینی فشار بخار برای فشارهای 100 و 10 کیلوپاسکال پرداخته شده است. همچنین با افزایش یک ترم به معادله اصلی و ارائه معادله کلی جدید بر پایه روش ریدل، خطای ناشی از پیش بینی مقدار فشار بخار برای فشارهای 100 و 10 کیلوپاسکال، کاهش داده شده است. پس از مشخص شدن معادله بهینه و معادله جدید، دقت معادلات با بررسی خطای حاصل از 40 ترکیب مختلف سنجیده شد. نتایج نشان داد که اصلاح اعمال شده بر معادله ریدل، خطاهای پیش بینی فشار بخار ترکیبات شیمیایی را کاهش می دهد.

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