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Modeling of Diffusion Coefficients for Binary Gas at P=101.325 kPa using Particle Swarm Optimization Algorithm

Amirhossein Oudi, Maryam Hosseini, Sara Azimi, Yegane Davoodbeygi *

1. Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Kashan, Iran. E-mail: amir95@grad.kashanu.ac.ir
2. Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Kashan, Iran. E-mail: aym.hosseini@gmail.com
3. Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Kashan, Iran. E-mail: sara.azimi93@alumni.kashanu.ac.ir
4. Department of Chemical Engineering, University of Hormozgan, Bandar Abbas, Iran. E-mail: y.davoodbeygi@hormozgan.ac.ir

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ABSTRACT

The diffusion coefficient of gases in a wide range of chemical processes is of great importance. Semi-empirical models for diffusion coefficient prediction are useful due to their relatively lower cost compared to laboratory methods. In this study, to facilitate the equations and accelerate the calculations, appropriate models have been presented using existing parameters such as molecular weight and critical properties to determine the binary diffusion coefficient of gases. The calculations have been performed using a particle swarm optimization (PSO) algorithm. This model has been used to obtain the diffusion coefficient of 84 gas dual systems at P=101.325 kPa and variable temperature (373.15-673.15 K). Also, during the validation phase, the suggested model attained the most accurate prediction with $R^2 = 0.9989$. This model is capable to predict the diffusion coefficient of gases with a mean relative error percentage of 2.57% and mean square error percentage of 0.15% compared to actual data. These results are significantly better than those obtained from other models.

Introduction

The diffusion coefficient in the phenomenon of mass transfer is of great importance for designing and simulation of different chemical processes [1]. As the theory and engineering applications of diffusional operations are advanced, increasing demands have arisen for diffusion coefficients of gases and vapors [2]. The diffusion of gases can be observed in many phenomena such as the movement of gases in the earth's strata, purification by adsorption, cooling of nuclear reactors, and permeability of various packing materials [3].

The relationship between the concentration gradient and the diffusion flux due to the concentration gradient is called Fick's law of diffusion, which is defined by the following Equations for binary mixtures:

$$J_1 = -CD_{12}\nabla x_1 \quad (1)$$

* Corresponding Author: Y. Davoodbeygi (E-mail address: y.davoodbeygi@hormozgan.ac.ir)

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$$J_2 = -CD_{21}\nabla x_2 \quad (2)$$

where each species is labeled by 1 or 2 subscripts. J_1 and J_2 (mole/cm^2.s) are the flux densities. C (mole /cm^2) is the total number density and the composition gradients are demonstrated in terms of mole fractions (x_1 and x_2). The diffusion coefficient is one of the key parameters in chemical processes. In binary mixtures, there is only one independent concentration gradient and one independent diffusion flux due to the survival of the total flux in the volume. As a result, the diffusion coefficients of Fick in binary mixtures are equal as follows [4]:

$$D_{12} = D_{21} \quad (3)$$

Numerous gases have had their diffusion coefficients measured over history and compiled. Table 1 shows an overview of the background of the studies conducted on the measurement and prediction of the diffusion coefficients of pure gases.

Table 1. A list of the techniques and correlations for diffusion coefficients

Source	Comment	Year	Ref
Camper et al.	This study introduces a brand-new semi-infinite volume method for calculating the diffusion coefficients of gases in ionic liquids at ambient temperature (RTILs). Henry's constants were measured using the same techniques as the diffusion coefficients. Along with the relationship of the diffusion coefficients with molecule size and viscosity, it is also examined how Henry's constants and diffusion coefficients relate to temperature. The gases used included carbon dioxide,ethylmethylimidazoliumbis (trifluoromethanesulfonyl)amide (emim), ethane, ethene, propane, and propane.	2006	[5]
Pillalamarry et al.	This essay examines the findings of an experimental investigation on the sorption and diffusion characteristics of methane in coals from the Illinois basin. First, the Langmuir Constants were estimated and the sorption findings were modeled using the Langmuir isotherm model. Next, the diffusion coefficient, D, was determined by modeling experimental data using the unipore diffusion theory and Fick's law of diffusion. For pressures lower than 3.5 MPa, the results unmistakably showed a negative link between D and pressure. It was discovered that the variation's overall pattern was bi-modal, with its value holding constant at high pressures and then rapidly increasing below this critical pressure. The findings of sorption and diffusion were compared, and the results showed that D was dependent on surface covering, which has a positive relationship with pressure. The results from previous studies using the bi-disperse diffusion model seemed to be in good agreement with the trend of diffusion variation with pressure. The practical implication of the findings is that methane migration is substantially facilitated by low pressures. This is a promising result given the low in situ pressure generally found in the Illinois basin. Finally, after several years of production, the San Juan basin's higher gas production rates may be caused, at least in part, by this tendency.	2011	[6]
Chen et al.	This study measures the methane diffusion coefficients in shale cores at supercritical circumstances using two different types of methane diffusion tests. According to experimental findings, (1) the free molecular diffusion coefficient is averaged out to be $1.214 \times 10^{-10}\,\frac{m^2}{s}$ under reservoir conditions from the isobaric diffusion experiments, but (2) the Knudsen diffusion, surface diffusion, and	2018	[7]

	configurational diffusion coefficients in the pressure decay experiments are more important for shale gas development. In matrix nanopores, where the mean diffusion coefficients are $4.99 \times 10^{-14} \frac{m^2}{s}$ for pores less than 4 nm and $9.03 \times 10^{-9} \frac{m^2}{s}$ for pores larger than 4 nm, it is shown that Knudsen diffusion and surface diffusion emerge simultaneously as gas transports. $2.06 \times 10^{-22} \frac{m^2}{s}$ is computed as the mean configurational diffusion coefficient for dissolved gas. To compare the theoretical results with the experimental data, the four types of diffusion coefficients indicated above are also theoretically estimated using the appropriate models. The relationship between gas diffusion and pore size is found by combining theoretical and experimental results, and this can help to further analyze the comprehensive diffusion behavior in shale gas development as well as the relative contribution of each diffusion during different production stages. This is because the measured methane diffusion coefficients correspond to a wide range of pore sizes. This work clarifies the behavior of gas diffusion throughout a range of pore sizes, which helps develop quantitative knowledge of the movement of shale gas in the matrix during production.		
Zhao and Jin	used molecular dynamics simulations to examine the diffusion coefficient of several gases in supercritical water. According to research, carbon monoxide has the slowest penetration while hydrogen has the fastest.	2020	[8]
Athar et al.	It has been discovered through soaking studies that the penetration of propane in heavy oil occurs in three stages: the early zone, the transition zone, and the late time zone. In all three areas, the coefficients of solubility and penetration of propane in the oil have been highly influenced by temperature.	2020	[9]
Zhao et al.	Molecular dynamics simulations have also been used to look into the diffusion coefficient of a particular group of gases in water at infinite dilution close to the critical point. To forecast the water permeability coefficient close to the critical point, a novel experimental equation has been proposed. The diffusion coefficient of all gases has been achieved with an average absolute relative error of 7.65%	2021	[10]
Si et al.	In this study, an improved model was built to account for both gas adsorption in residual pores and gas dissolution in pore water when calculating the effective diffusion coefficient of the gas in a water-saturated coal core. Since the traditional model only takes into account the gas dissolution in pore water, the calculation results of the improved model using a PVT (Pressure-Volume-Temperature) test method are in the range of 1.03×10^{-12} to$30.40 \times 10^{-12} \frac{m^2}{s}$, which are 5 to 6 orders of magnitude lower than those calculated by the traditional model. As a result, the findings of the revised model are closer to reality. Additionally, tests including saturated moisture, equilibrium moisture, and NMR were conducted. Results indicate that equilibrium and saturated moisture both decline with increasing coal rank. As the coal rank rises, the pore size transitions from micropore/mesopore-dominated to micropores-dominated. Additionally, the fraction of open porosity gradually declines as the coal rank rises, whereas the proportion of closed porosity rises, suggesting that pore connectivity declines as the coal rank rises. The effects of pore structure, pressure, liquid characteristics, and adsorbability on the effective diffusion coefficient were then examined.	2021	[11]

An et al.	In this study, the diffusion coefficients under varied stress, concentration gradient, temperature, and gas-type circumstances were obtained using a direct steady-state technique based on Fick's law. It is discovered that the stress and the gas diffusion coefficient have a weak negative linear association. While the diffusion coefficient of non-adsorptive gas (helium) decreases first and then increases, the diffusion coefficient of methane decreases in a power function as the concentration gradient grows. The Arrhenius formula is satisfied by the gas diffusion coefficient in coal, which exhibits a positive correlation with temperature. In order to forecast the characteristics of coal's gas desorption with changing temperatures, a model taking diffusion coefficient variation for coal particles into account was developed based on the measured relationships and Fick's law. The dependability of the direct measurement method of the diffusion coefficient is demonstrated by the agreement between the expected and measured results. It might offer a fresh approach to predicting the behavior of gas diffusion in coal under varying circumstances.	2022	[12]
Chen et al.	The first thing this research did was present a back propagation (BP) neural network-based quick and easy prediction approach for diffusion coefficient for both CO_2-oil systems within and outside of porous media. 18.73% and 18.80% of the errors are on average, respectively. Models can be regularly updated to produce more precise estimations of the supercritical CO_2-oil system without/with porous medium conditions with the ongoing addition of new data. The correlation between the diffusion coefficient and temperature, pressure, permeability, porosity, and surface area is positive. The volume of porous media, oil density, and oil viscosity all negatively correlated with the diffusion coefficient. It is important to remember that for rocks with a certain volume, an increase in surface area can greatly increase the diffusion coefficient, implying that a direct upscale of the CO_2 diffusion coefficient determined in the lab is completely irrational.	2022	[13]
Bellaire et al.	For all mass transfer processes, diffusion coefficients at infinite dilution are crucial fundamental information. They can be discovered by utilizing nuclear magnetic resonance spectroscopy with pulsed field gradients (PFG-NMR), a method that is frequently used in chemistry but is only occasionally employed in engineering studies, to analyze substances that are in equilibrium. Here, at 298.15 K, the self-diffusion coefficients of diluted solutions of carbon dioxide and methane in the pure solvents water, ethanol, cyclohexane, toluene, methanol, and acetone were measured using this useful method. Measurements were also made for the systems (carbon dioxide + water) and (carbon dioxide + ethanol) at 308.15 K, 318.15 K, and 333.15 K. No literature data were previously available for the methane-containing systems, with the exception of (methane + water) and (methane + toluene). At the studied solute concentrations, there is almost no difference between the self-diffusion coefficient and the mutual diffusion coefficient. To predict diffusion coefficients at infinite dilution, the experimental results are compared to experimental literature data as well as to findings from semi-empirical approaches. Additionally, using force fields that were collected from the literature, molecular dynamics simulations of all systems were run to calculate the diffusion coefficient at infinite dilution. The results	2022	[14]

are then compared to the experimental data and those from the traditional prediction methods.

When the complication issues rise, the experimental data must be estimated. Traditional optimization algorithms may be hard to meet the supplies of the problems so leading to new influential algorithms [15]. Over the past few years, various traditional novelty algorithms have been developed as impressive and practical approaches to problem optimization [16, 17]. Due to the continuous improvement of computing power. By using numerical integration, they aimed to quickly optimize the reaction rate, and conversion range, and accommodate any collection of differential rate equations [18]. Particle swarm optimization (PSO) and genetic algorithm (GA) are the most hopeful algorithms for network optimization [19]. PSO as an evolutionary random algorithm that is nature-inspired is evoked by the public behavior of organisms, which warrants a coordinated swarm to achieve the ideal result extended by Kennedy and Eberhart [20]. It is randomly placed in the workspace, and each particle's objective function quantity is assessed [21]. Like GA, PSO is an optimization tool that is based on population. But, GA and PSO are different in some ways: (1) PSO has a various evolutionary mechanism, with the exception of genetic agents such as crosses and mutations, which update their PSO particles at internal speeds. (2) At the same time, particles of PSO have a memory that is vital for the algorithm [22].

In recent years, the optimization algorithm PSO was used the nonlinear Regression in problems such as, Model design and parameter estimation for the thermodynamics, kinetics, and hydrodynamics of mixed salt precipitation in porous media [23], Interacting parameter correlation in the Wilson, NRTL, and UNIQUAC models [24], toxic vapors' kinetic adsorption on activated carbon in the batch reactor [25], predict crude oil properties [26], For the gas cross flow in packed bed reactors, a novel Sauter mean diameter correlation has been developed [27], and An innovative theoretical and practical approach based on friction volume theory and friction theory parameter tweaking for viscosity-sensitive Iranian heavy crude oils [28].

In previous studies, relationships have been proposed to obtain the diffusion coefficient, which is mostly complex and detailed, and there are some difficulties in using them. In this study, an optimum and simple model with a low error rate of specific gases is proposed by Particle Swarm Optimization (PSO) using data related to the physical properties of gas in P=101.325 kPa.

Methodology

PSO Algorithm

James Kennedy and Russell Eberhart presented the particle swarm optimization technique in 1995. This algorithm is adapted from the collective performance of a collection of animals such as fliers and fish [29]. PSO is an optimization approach based on population inspired by the public treatment of birds or fish training. It sometimes bears many similarities to Evolutionary Calculation techniques (EC), Genetic Algorithms (GA), and Evolutionary Strategies (ES). But there are also many contrasts between these methods [30]. The PSO starts with a collection of chance iotas (solutions) and therefore takes optimal search by keeping generations up to date by coursing the best valuations in every entrance, in which every particle is kept up to date. The first of these values is the foremost fit ($x^{i,pbest}[t]$). This foremost value is the best value in the world and is entitled ($x^{gbest}[t]$). After gaining the two foremost values, the particle keeps its velocity and position of itself up to date by means of the following equations:

$$v^i[t+1] = wv^i[t] + c_1r_1(x^{i,pbest}[t] - x^i[t]) + c_2r_2(x^{gbest}[t] - x^i[t]) \quad (4)$$

$$x^i[t+1] = x^i[t] + v^i[t+1] \quad (5)$$

The $x^i[t+1]$ and $v^i[t+1]$ is the position and velocity of the particle "i" in the new iteration. The $x^{i,pbest}[t]$ shows the foremost position of particle" i", and $x^{gbest}[t]$ represents the foremost position among the whole available particles. r_1 and r_2 are the random number between zero and one. c_1 and c_2 are positive constant parameters entitled acceleration coefficients. w is the inertia weight that is used to ensure convergence. Fig. 1 shows the flowchart algorithm for particle swarm optimization [31].

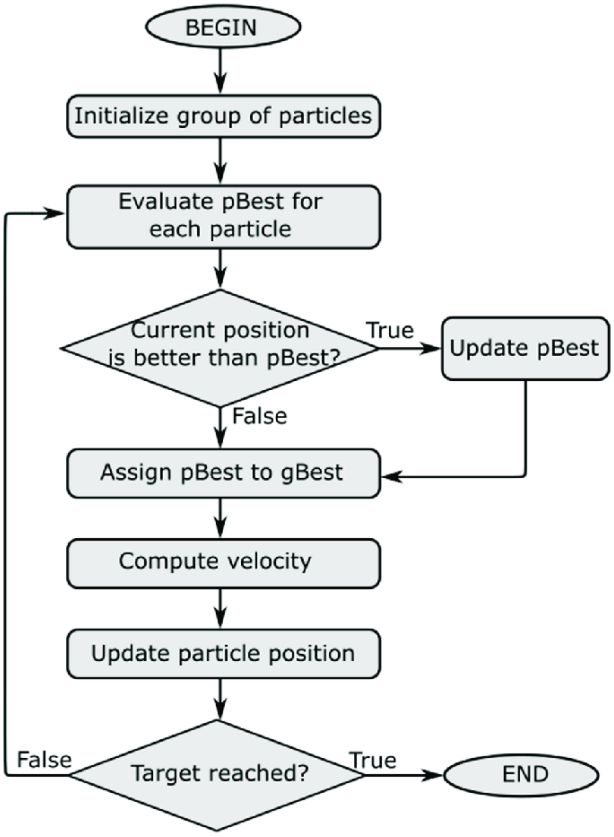

Fig. 1. Flowchart algorithm for particle swarm optimization

The optimal amounts of the parameters w, c_1 and c_2 are obtained from the following relations. Table 2 specifies the implementation parameters of the particle swarm optimization algorithm.

$$K = \frac{2k}{\emptyset - 2 + \sqrt{\emptyset^2 - 4\emptyset}} \quad (6)$$

$$\emptyset = \emptyset_1 + \emptyset_2 \quad (7)$$

$$w = K \quad (8)$$

$$c_1 = K\emptyset_1 \quad (9)$$

$$c_2 = K\emptyset_2 \quad (10)$$

In the above equations, $\emptyset_1$ and $\emptyset_2$ are constant values greater than zero, respectively, which must be adjusted to achieve the optimal value of the parameters of the particle swarm algorithm,

including inertial coefficient (w), and learning coefficients (c_1 and c_2). Clerk suggested that if the values $\emptyset_1$ and $\emptyset_2$ were equal to 2.05 and the value of K was considered equal to one, the optimal value of 0.73 for the inertial coefficient would be obtained [32]. The PSO is employed for data fitting issues, at which the variables are the required coefficients of the regression model for data fitting. In the case of a randomly initialized solution at the first iteration, we can calculate the minimized error between the actual output value and predicted value from initialized solution to compute the fitting function. $a_0^{i.k}$, $a_1^{i.k}$, ..., $a_n^{i.k}$ can be considered as the solution resulting from the PSO for i iteration and k population. The predicted output value related to $a_0^{i.k}$, $a_1^{i.k}$, ..., $a_n^{i.k}$ for both the linear and non-linear regression models can be obtained using the following equations [33]:

$$y_{Predicted} = a_1^{i.k}x_1 + a_2^{i.k}x_2 + \cdots + a_n^{i.k}x_n + a_0^{i.k} \quad (11)$$

$$y_{Predicted} = a_n^{i.k}x_n + a_{n-1}^{i.k}x_{n-1} + \cdots + a_1^{i.k}x_1 + a_0^{i.k} \quad (12)$$

To generate the fitness function, can be used is assessed by the equation below [34]:

$$E_i = \sum_{j=1}^{n}(P_{ij} - T_j)^2 \quad (13)$$

where T_j is the desired value for fitness case j and P_{ij} is the value predicted by the individual program i for fitness case j (out of n fitness instances).

Table 2. Parameters of the particle swarm optimization algorithm

Parameter	Value
Number of Iterations	2000
Population size	100
Mutation	0.04
Internal coefficient(w)	0.7298
Personal learning coefficient(c_1)	1.4962
General learning coefficient(c_2)	1.4962

Data Acquisition and Analysis

Experimental diffusion coefficient data for 84 systems at P=101.325 kPa and different temperatures have been selected [35] as the basis for comparison in determining the relative accuracy of the PSO algorithm method. The physical properties of pure gases including temperature, critical temperature, critical volume, and molecular weight were obtained from laboratory data and used for the prediction of the diffusion coefficient of these gases.

Selection of Optimal Configuration

Three crucial characteristics that affect how well the constructed model performs are defined in this section. Each input data's correlation coefficient serves as the parameter [36]:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(D_{exp} - D_m)^2}{\sum_{i=1}^{n}(D_{exp} - \bar{D}_{exp})^2} \quad (14)$$

The second is the mean square error (MSE) [37]:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(D_{exp} - D_m)^2 \quad (15)$$

The third parameter is the mean relative error (MRE) [38]:

$$MRE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{D_{exp} - D_m}{D_{exp}}\right| \quad (16)$$

n is the number of data points, D_{exp} is the experimental diffusion coefficient, $\overline{D}_{exp}$ is the average value of the experimental values and D_m is the diffusion coefficient obtained from the modeling.

Results

The general model for the constant prediction of diffusion coefficients for binary gas mixtures at atmospheric pressure is:

$$D_{12} = \frac{a_0 T^{a_1}\left(\frac{1}{Mw_1} + \frac{1}{Mw_2}\right)^{a_2}}{P(T_{c1}T_{c2})^{a_3}(V_{c1} + V_{c2})^{a_4}} \quad (17)$$

Eq. 17 was created using the PSO algorithm method. Using this equation, the diffusion coefficient of gases can be calculated with less error. This equation is based on the temperature, pressure, and physical properties of the material. a_0, a_1, a_2, a_3 and a_4 are fixed coefficients and the related numerical values are given in Table 3.

Table 3. Correlated constants for determination of the diffusion coefficient.

Constant	Value
a_0	0.3575
a_1	1.7335
a_2	0.5335
a_3	0.1061
a_4	0.6455

The correlation between the simulation results is shown in Fig. 2.

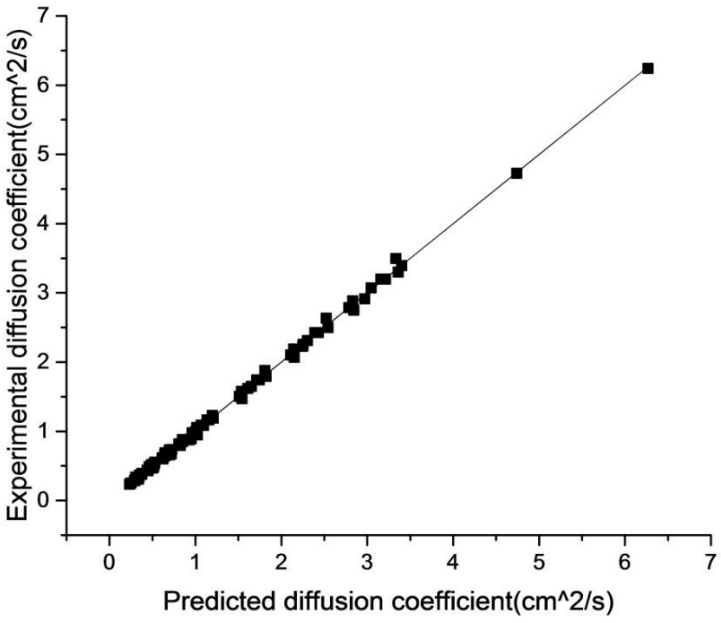

Fig. 2. Correlation of experimental data versus PSO predictions

Table 4 shows the MRE, MSE and R^2 values calculated.

Table 4. The MRE, MSE and R^2 values for the PSO configurations

MRE×100	MSE×100	R^2
2.57	0.15	0.9989

Table 5 shows the binary systems used in this model along with the mean relative error. Comparison of the method with experimental data shows that the PSO algorithm method provides acceptable results for the diffusion coefficient so the highest and lowest error rate in this model is 8.9% and 0%, respectively.

Table 5. Correlated results for determination of the diffusion coefficients.

Name	T (K)	RE(%)	Name	T (K)	RE(%)
Ar-CH_4	373.15	8.75	CH_4-O_2	573.15	1.20
Ar-CH_4	473.15	7.55	CH_4-O_2	673.15	1.74
Ar-CH_4	573.15	6.58	CO-H_2	373.15	2.25
Ar-CH_4	673.15	5.64	CO-H_2	473.15	1.65
Ar-CO	373.15	0.36	CO-H_2	573.15	1.36
Ar-CO	473.15	0.06	CO-H_2	673.15	1.17
Ar-CO	573.15	0.42	CO-He	373.15	3.19
Ar-CO	673.15	0.70	CO-He	473.15	2.53
Ar-CO_2	373.15	0.62	CO-He	573.15	2.05
Ar-CO_2	473.15	3.43	CO-He	673.15	1.73
Ar-CO_2	573.15	4.94	CO-N_2	373.15	8.91
Ar-CO_2	673.15	5.74	CO-N_2	473.15	5.92
Ar-H_2	373.15	2.38	CO-N_2	573.15	4.30
Ar-H_2	473.15	3.56	CO-N_2	673.15	3.06
Ar-H_2	573.15	4.23	CO-O_2	373.15	0.01
Ar-H_2	673.15	4.64	CO-O_2	473.15	0.28
Ar-He	373.15	1.77	CO-O_2	573.15	0.46
Ar-He	473.15	0.25	CO-O_2	673.15	0.55
Ar-He	573.15	1.03	CO_2-H_2	373.15	8.10
Ar-He	673.15	2.09	CO_2-H_2	473.15	4.99
Ar-N_2	373.15	2.09	CO_2-H_2	573.15	4.15
Ar-N_2	473.15	1.78	CO_2-H_2	673.15	3.59
Ar-N_2	573.15	1.30	CO_2-N_2	373.15	0.80
Ar-N_2	673.15	1.02	CO_2-N_2	473.15	3.37
Ar-O_2	373.15	4.24	CO_2-N_2	573.15	4.50

Table 6. Continued correlated results for determination of the diffusion coefficients

Name	T (K)	RE(%)	Name	T (K)	RE(%)
Ar-O_2	473.15	4.27	CO_2-N_2	673.15	4.78
Ar-O_2	573.15	4.19	CO_2-O_2	373.15	0.66
Ar-O_2	673.15	4.18	CO_2-O_2	473.15	0.85
CH_4-H_2	373.15	1.04	CO_2-O_2	573.15	1.81
CH_4-H_2	473.15	0.31	CO_2-O_2	673.15	2.22
CH_4-H_2	573.15	0.27	H_2-He	373.15	0.06
CH_4-H_2	673.15	0.79	H_2-He	473.15	0.22
CH_4-He	373.15	1.07	H_2-He	573.15	0.35
CH_4-He	473.15	0.75	H_2-He	673.15	0.40
CH_4-He	573.15	0.42	H_2-N_2	373.15	0.49
CH_4-He	673.15	0.15	H_2-N_2	473.15	0.12
CH_4-N_2	373.15	7.86	H_2-N_2	573.15	0.42
CH_4-N_2	473.15	7.51	H_2-N_2	673.15	0.61
CH_4-N_2	573.15	7.23	H_2-O_2	373.15	1.73
CH_4-N_2	673.15	6.83	H_2-O_2	473.15	1.79
CH_4-O_2	373.15	1.34	H_2-O_2	573.15	1.85
CH_4-O_2	473.15	0.28	H_2-O_2	673.15	1.87

To evaluate the performance of the proposed model in comparison with other models [39-43], the amounts of errors obtained from each model are shown in Fig. 3. It is found that the proposed model with a mean relative error of 2.57% has less error in predicting the diffusion coefficients compared to other models.

Generally, the results obtained from the proposed model are in good agreement with the experimental results. It is worth mentioning that most of the previous models proposed to determine the double diffusion coefficient of gases have variables that require extensive information such as knowledge of the collision diameter between gas molecules, intermolecular forces, and liquid molar volume at normal boiling point. Also, the required parameters for these equations are available for a limited number of materials. However, our proposed model is based on the critical properties that are available for most components. Generally, our study demonstrates the employment of an appropriate modeling method that is applicable for predicting the penetration coefficient of gases which is advantageous for the simulation of chemical processes in the industry.

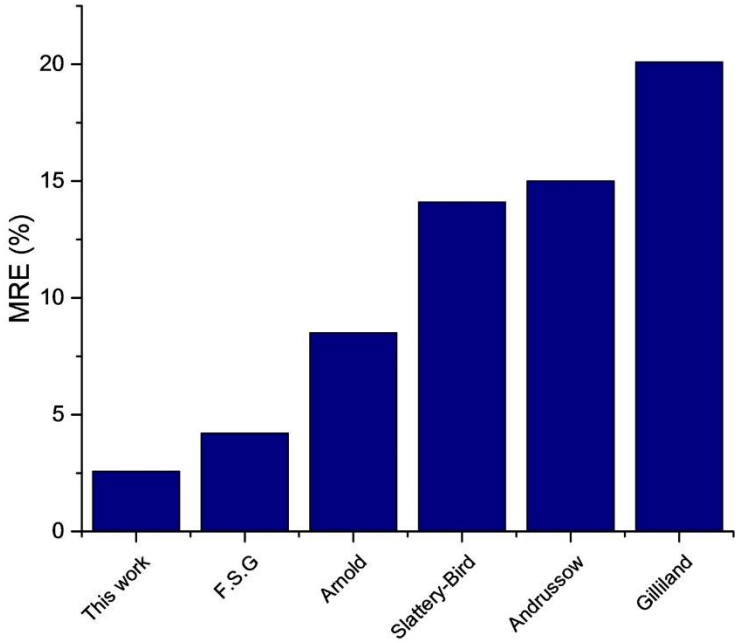

Fig. 3. Comparison between errors obtained from our proposed method with those of previous models

Conclusion

In this study, a semi-empirical equation has been obtained using the PSO algorithm to calculate the binary diffusion coefficient of gases for various systems at P=101.325 kPa and variable temperatures. In order to forecast the diffusion coefficient of these gases, the physical parameters of pure gases, such as temperature, critical temperature, critical volume, and molecular weight, were acquired from laboratory data. During the validation phase, the suggested model attained the most accurate prediction with $R^2 = 0.9989$, MRE=2.57% and MSE=0.15%. The result of our study is advantageous for the simulation of different chemical processes based on gases through appropriate prediction of the diffusion coefficient. It is important to note that the majority of the earlier models that were suggested to figure out the double diffusion coefficient of gases contain variables that call for a lot of background knowledge, like understanding gas molecule collision diameters, intermolecular forces, and liquid molar volumes at normal boiling points. Additionally, only a few materials have the

available parameters for these equations. Our suggested model, however, is based on the essential characteristics that are present in the majority of components.

Nomenclature

D_{12}	diffusion coefficients ($\frac{Cm^2}{s}$)
Mw	Molecular weight
P	Pressure (kPa)
T	Temperature (K)
T_c	Critical Temperature (K)
V_c	Critical Volume ($\frac{m^3}{mol}$)

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