Research article

Prediction of methane diffusion coefficient in water using molecular dynamics simulation

Hojatollah Moradi [a], Hedayat Azizpour [a,b,*], Hossein Bahmanyar [a,**], Mohammad Mohammadi [a], Mahdi Akbari [a]

[a] Surface Phenomenon and Liquid-Liquid Extraction Research Lab, School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran
[b] Department of Chemical Engineering, Fouman Faculty of Engineering, College of Engineering, University of Tehran, Iran

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ABSTRACT

Diffusion coefficient is one the most effective factors in mass transfer calculation, which plays an important role in study at the molecular scale. In this study, Material Studio software was used to simulate the diffusion coefficient of methane in water through molecular dynamics. COMPASS force field was also used for optimization of atomic structures of methane and water, and Group-Based method was applied to model to calculate both van der Waals and electrostatic forces. In addition, Universal force field was used to optimize of amorphous cell, while Ewald and Atom-Based methods were applied for modeling and calculation of van der Waals and electrostatic potential energy at constant temperatures. The simulation duration for equilibrium of amorphous cell in both state of NVT and NVE was assumed 5ps. The impact of temperature as well as concentration on diffusion coefficient were investigated and results showed that the diffusion coefficient had linear relationship with temperature and third-degree polynomial relationship with concentration. As a result, of the simulation, the diffusion coefficient function versus temperature and concentration was developed.

1. Introduction

The diffusion coefficient in liquids is an important parameter to discover not only the mechanism of complicated mass transfer phenomenon but also to design different types of separation columns such as distillation and adsorption column [1]. In particular, the infinite dilution diffusion coefficient of solute (component 1) in solvent (component 2) abbreviated as D_{12}, is one of the most important transport features in velocity-controlled processes [2, 3, 4]. The diffusion coefficient for a particular chemical system can be obtained experimentally but the procedure comes at a huge cost and takes a lot of time as well. There are a number of models calculating the diffusion coefficient in liquids, neither of which has the ability to predict the diffusion coefficient of systems containing only one liquid component [5]. Most of the presented models are based on the Stokes-Einstein model [6]. In 2002, Kooijman developed a model based on Stokes-Einstein theory that reduced the error by 10% [7]. The quality of a model is measured by comparison with experimental values; the lower difference between the predicted and the experimental values, the better accuracy of the model. In recent years, due to costly

prolonged procedure of experimental data acquiring and significant error of presented models, the calculation of diffusion coefficient using molecular dynamics simulation has attracted much attention. The experimental molecular diffusion coefficients in studies are slightly different from the results of simulation with molecular dynamics, which can be due to distinct in the samples and the corresponding methods [8, 9]. Kang et al. reported methane diffusion coefficient in kaolinite [10] as an example of the difference.

Gao et al. [11] used the Materials Studio software package to simulate the adsorption and diffusion of Nitrogen, Methane, Water and Carbon Dioxide into micropores of lignite in which Einstein equation was used to calculate the diffusion coefficient. In this study, the Ewald Group-basedmethod with accuracy of 0.001 kcal/mol was used to calculate the electrostatic potential, while the Atom-based summation method with the cutoff truncation of 1.25 nm used for van der Waals interactions as well.

In addition, in the study of JingHua Tan et al. [12], the diffusion and adsorption process of five gases N2, H2, CH4, CO2 and O2 in hydrogenated nitrile butadiene rubber (HNBR) and ethylene-propylene-diene

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rubber (EPDM) were simulated by Molecular Dynamics Simulation. The diffusion coefficients of all gases except CO2 in HNBR and EPDM molecules are related to the diameter of effective diffusion. Because of linearity, CO2the lowest diffusion coefficient. Also, the interaction between CO2 and HNBR increases the coherence between the chains due to the presence of –CN polar groups in the HNBR chains and shows a lower diffusion coefficient range than EPDM.

The dependence of molecular diffusion coefficient on mass transfer operations is often underestimated, while this factor plays an important role in the transfer study of gases into liquids. Khalifi et al. [13] investigated the effect of different concentrations of Ethane on the molecular diffusion coefficient of this gas in liquid Toluene. The results proved that there is a significant dependence on the concentration of the gas in the liquid mixture. They used the obtained data to investigate the dependence impact of molecular diffusion coefficient on concentration in mass transfer of ethane in toluene. Findings also revealed that the assumption of a constant diffusion coefficient introduces 10%–60% error in calculation of diffusional mass transfer flux in the ethane-toluene system.

The purpose of the study is to investigate the accuracy and possibility of using molecular dynamics simulation to calculate the molecular diffusion of methane in water, as well as comparing experimental and simulated results by molecular dynamics. Moreover, the impact of temperature and concentration on the molecular diffusion coefficient was investigated to find an appropriate equation.

2. Models and method

Application of computational methods using computer simulation has had a significant effect on our awareness about Nano-fluids behavior and the physical phenomena occurring on molecular scale. In addition, when it is not possible to conduct laboratory tests in some cases, computer simulations can be used instead. Molecular dynamics is one of the computer simulation techniques that is based on the interaction between atoms and molecules. It solves the Newton's equations of motion for particles using the theory of atomic motion in a period of time to measure their pathway, while the particles force field and potential energy is determined by applying atomic potential or molecular mechanics force field [14, 15, 16, 17, 18]. Also, molecular dynamics can give us a physical data set, such as diffusion coefficient, viscosity, adsorption, etc. [19, 20].

In this study, diffusion process of methane in water was simulated by Molecular Dynamics Simulation method at different temperature and concentration. Materials Studio software was used for molecular dynamics simulation to calculate the molecular diffusion coefficient of methane in water. Initially, the structure energy of water and methane molecules were optimized before production of cells, and an optimized structure was used for molecular simulation and diffusion. The COMPASS[1] force field was applied for optimization of water and methane atoms. A Group-Based integration method was used to model and calculate the potential energy of van der Waals and electrostatic energy. Having formed the structure of water and methane atoms, the Universal force field was used to optimize the amorphous cells. In addition, Ewald and Atom-Based integration method were applied for modeling and calculation of the electrostatic and van der Waals energy potential at constant temperatures. In a study done by Zhaoal [21]. about the impact of system resizing by changing amorphous cell dimensions in three different size of 30, 50 and 70 Å, it was concluded that the dimensions had negligible effect on predicting the diffusion coefficient. One molecule of methane in 1000 molecules of water for a concentration of 0.1 wt % was used to make the amorphous cell. Besides, the cell was optimized in the temperature range of 290–500 K. In Table 1, the number of CH_4 and H_2O molecules and the resulting concentration is shown in each cell

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[1] Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies.

dimension. For example, amorphous cell dimension for weight fraction of 0.1% was assumed as 3.11 nm × 3.11 nm × 3.11 nm.

In order to reach the equilibrium state, Canonical ensemble (NVT) was initially applied for 5 ps on system. Chemical potential (μ), volume (V) and temperature (T) are were considered as constant amounts during the simulation and it is assumed that the framework is in contact with a tank by infinite temperature and pressure [22, 23]. Finally, Micro-Canonical ensemble (NVE) was applied on system at temperatures of 293, 298, 303.05, 308.25, 315.75 and 320 K adjusted by Langevin thermostat for 5 ps to reach the equilibrium [24, 25]. The application of the NVE ensures that dynamic properties such as scattering coefficients are not biased by the system-wide algorithms used to generate a constant temperature set [26, 27]. To calculate the diffusion coefficient according to Eq. (1) in which there is a linear relationship between MSD and time, Mean Square Displacement abbreviated as **MSD** was used [28]:

$$D = \frac{1}{6N_a} \lim_{t \to \infty} \frac{d}{dt} \sum_{i=1}^{N_a} [r_i(t) - r_i(0)]^2 \tag{1}$$

Where $N_a$is the number of dispersed atoms in system and $r_i(t)$ is the displacement vector of the i molecule at time of t. MSD diagram versus time can be drawn to calculate diffusion coefficient by plotting the best line (y = a×x + b) passes through the points. Diffusion coefficient can be obtained by Eq. (2) [29]:

$$D = \frac{a}{6} \tag{2}$$

2.1. Force field and model validation

The simulation results compared with reported experimental data by Witherspoon and Saraf [30] who measured diffusion coefficient of methane in water at 298, 305.25 and 315.74 K (Table 2). Firstly, the diffusion coefficient of methane in water was simulated at these temperatures, then, the accuracy of method was confirmed by comparison of obtained result-D_{AB}^{sim} (cm^2/s)- with experimental data-D_{AB}^{Exp} (cm^2/s)- in Eq. (3).

$$Erorr(\%) = \left(\frac{D_{AB}^{Exp} - D_{AB}^{sim}}{D_{AB}^{Exp}} \right) \times 100 \tag{3}$$

In addition, comparison of D_{AB}^{sim} and D_{AB}^{Exp}revealed the reported force field data and that were significant in the model and could be used to measure temperature and concentration effects.

Moreover, in order to validate the accuracy of simulation result, calculation of theoretical diffusion coefficient was implemented by Wilke-Chang equation [31]. This equation was used to calculate the diffusivity of CH_4 and H_2O [32]. Eq. (4) shows the Wilke-Chang equation.

$$D_{AB} = 1.173 \times 10^{-16} (\varnothing M_B)^{0.5} \frac{T}{\mu V_A^{0.6}} \tag{4}$$

M_B: Molecular Weight of solvent B (kg/kmol)
μ = Viscosity of solvent B (kg/ms)
VA = Molar Volume of solute at the boiling point (m^3/kmol)
$\varnothing$ = Association parameter for solvent, 2.26 for water
T = Temperature of system (K)

A comparison between experimental and simulated data, as well as theoretical results can be made from Table 2 and Figure 1. The MD simulation results are closer to experimental data.

Figure 2 shows the line graphs for MSD versus time at four distinct temperatures of 293 K, 303.05 K, 308.25 K and 315.75 K regarding the procedure that Masiren et al. and Gautieri have already described in which line graphs of MSD versus time were used for calculation of diffusion coefficient [18, 33]. Thus, according to Figure 2, linear increase

Table 1. Characteristics of Amorphous cell.

C (ppm)	H$_2$O	CH$_4$	a×b×c (nm)
300	3333	1	4.64×4.64×4.64
400	2500	1	4.21×4.21×4.21
500	2000	1	3.91×3.91×3.91
1000	1000	1	3.11×3.11×3.11
1500	677	1	2.73×2.73×2.73
2000	500	1	2.47×2.47×2.47
2500	400	1	2.29×2.29×2.29

Table 2. Reported diffusion coefficient of methane in water at 298, 305.25 and 315.74 K [30].

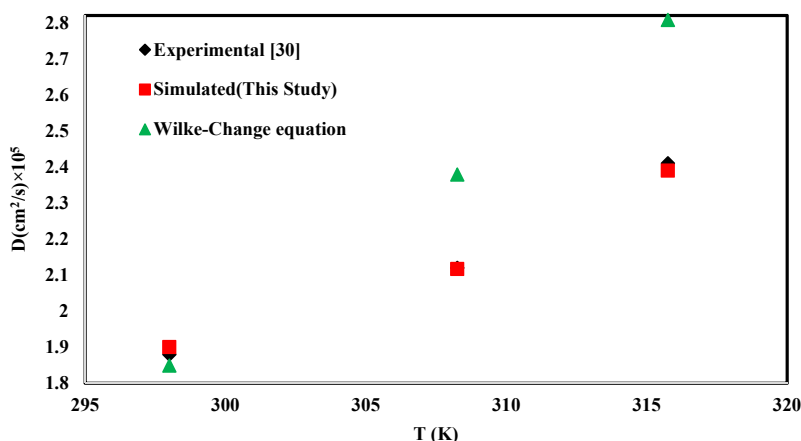| T(k)	D_{AB}^{Exp} (cm^2/s)×10^5	D_{AB}^{MD} (cm^2/s)×10^5	Error (%) (MD)	D_{AB}^{WC} (cm^2/s)×10^5	Error (%) (WC)
298	1.88±0.01	1.90013	-1.7	1.8489	1.65
308.25	2.12±0.03	2.11698	0.142	2.3786	-12.19
315.75	2.41±0.02	2.38968	0.843	2.80776	-16.504

Figure 1. Diffusion coefficient of methane in water versus temperature with a concentration of 1000 ppm.

in the slope of MSD graphs versus time [34] indicates a rise in temperature as well [18]. The more temperature rises, the size of the box increases and make the atoms move faster. Zhao et al. [21] conducted a research on the diffusion of methane in supercritical water at the temperature of 673–973 K and the pressure of 250 atm. As the temperature increased, the slope of the MSD line increased and they found that the MSD graph fluctuated more at higher temperatures although there is no change in the tendency to be linear.

2.2. Effect of temperature on diffusion coefficient of methane in water

One of the basic equations to determine the diffusion coefficient of gas in liquids is the Stokes-Einstein equation [35] According to which, the diffusion coefficient is directly proportional to the absolute temperature:
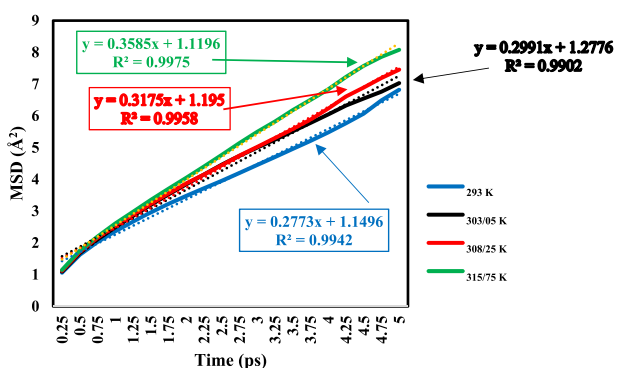

Figure 2. Prediction of diffusion coefficient graph for methane in water at 293 K, 303.05 K, 308.25 K and 315.75 K.
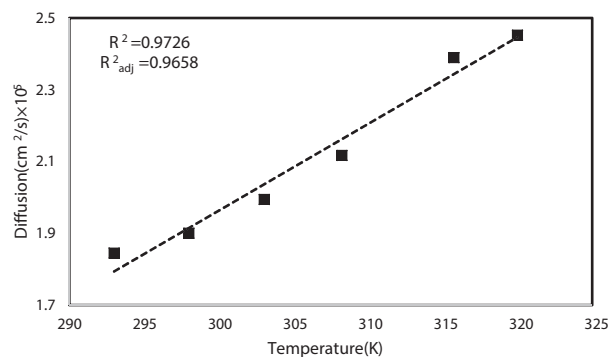

Figure 3. Diffusion coefficient of methane in water versus temperature at constant weight percent of methane (0.1%).
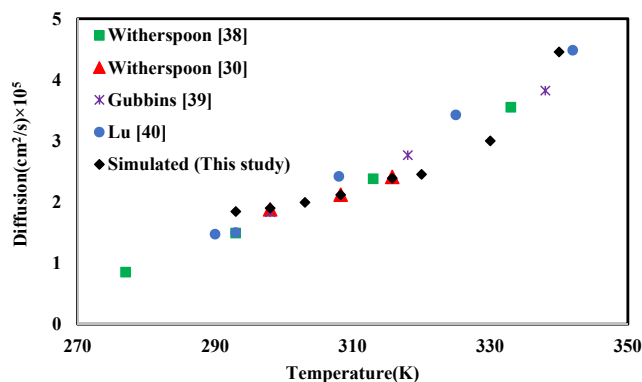
Figure 4. Diffusion coefficient of methane in water versus temperature at constant pressure of 100 kPa.
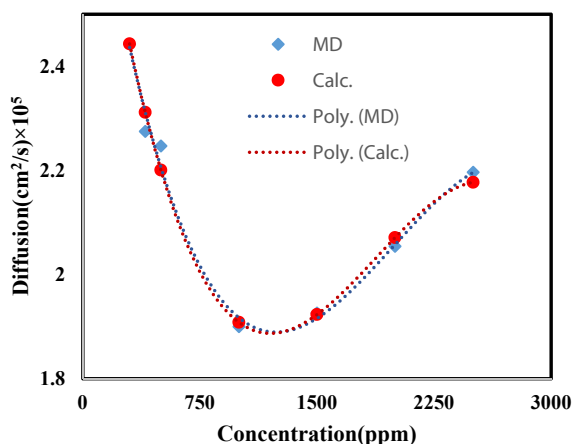

Figure 5. Molecular dynamics simulated and calculated diffusion coefficient of methane in water at T = 298 K.

$$D = \frac{R}{6N_A \pi \eta_a} T \qquad (5)$$

As the temperature increases, the mean kinetic energy of the gas molecules increases, which leads to a rise in the velocity of the molecules. The more speed enhances, collision between the molecules and better diffusion as a result is more likely to happen. Khane Athar et al. [36] calculated the diffusion coefficient of propane gas in heavy oil at high temperatures. In this study, the diffusion coefficient increased linearly with rise in temperature. In the heating process, the viscosity of the heavy oil reduces, which causes an enhancement on the diffusion coefficient of propane in the heavy oil based on the Stokes-Einstein equation.

In addition to a similar result reported for methane diffusion [9], Molecular motion of gas enhances by rising the temperature and causes an increase in diffusion coefficient as well [10]. Figure 3 shows the

Table 3. The Molecular Dynamics simulated and calculated for diffusion coefficient of methane in water at T = 298 K.

C (ppm)	$D_{AB}^{MD}(\text{cm}^2/\text{s}) \times 10^5$	$D_{AB}^{Calc}(\text{cm}^2/\text{s}) \times 10^5$
300	2.44276	2.443087
400	2.275016	2.31165
500	2.246983	2.200888
1000	1.90013	1.908341
1500	1.92625	1.92325
2000	2.05433	2.071096
2500	2.196516	2.067516

Table 4. Comparison of R^2 for molecular dynamics simulated and calculated diffusion coefficient of methane in water.

	MD	Calc.
R^2	98.53	98.24624
R^2_{adj}	-	96.93092
R_{MSD}	-	0.0081311
Variance	-	0.0010578

impact of temperature on diffusion coefficient of methane in water at constant concentration. It has been proved that the diffusion coefficient linearly increases at higher temperatures with regard to Eq. (6):

$$D_{AB}^{MD} = 0.0242T - 5.2911 \qquad (6)$$

Furthermore, Vasileios et al. [37] predicted the diffusion of methane into water. At a pressure of 0.1 MPa and the temperature range of 273–360 K, the diffusion coefficient increased linearly. while at pressures of 5 and 20 MPa and higher temperatures, the linear mode changed to the curved graph. Mr. Zhao et al. [21] have also achieved similar results in the temperature range of 673–973 K and pressures of 250, 265 and 280 atm.

In addition, the given Figure 4 is the illustration of diffusion coefficient of methane in water as a function of temperature at a constant pressure of 100 kPa, and there is a comparison between experimental and simulated data [30, 38, 39, 40]. In all cases, the diffusion coefficients increase with rise in temperature for liquid soluble gases [4]. Figure 4 also shows that the Universal force field provides an appropriate agreement between the experimental data and simulation results for the studied systems and conditions.

2.3. Effect of concentration on diffusion coefficient of methane in water

Although methane concentration has complicated impact on diffusion coefficient, investigation of its reliance is a key factor for understanding the mechanism of diffusion phenomena through modeling [36]. Figure 5 indicates the influence of concentration on diffusion coefficient at constant temperature of 298 K. Having increased the concentration from 300 ppm to 1000 ppm, diffusion coefficient initially reduced while it enhanced from 1000 ppm to 2500 ppm. Therefore, diffusion coefficient of methane in water has a minimum value at 1000 ppm and this fact has been discussed in several researches [41, 42]. Moreover, Eq. (7) shows a correlation between diffusion coefficient of methane in water and concentration that follows third order in which the R^2 equals to 98.53%. In addition, Eq. (7) was obtained as a result of using molecular dynamics simulation for prediction of diffusion coefficient, while Eq. (8) measures the calculated value of this parameter. Table 3 and Figure 5 show the simulation and calculated findings. Differences in R^2 between Eqs. (8) and (9) are presented in Table 4 which indicates a significant similarity. The decline in both MD and Calc. lines has been attributed to a decrease in the mean leap distance, since there are more frequent collisions at higher concentrations [42]. In Darken relation, several groups were assumed responsible for the enhancement of both MD and Calc. curved lines [43, 44, 45]. This approach is based on the empirical models relating the mutual diffusion coefficients to the self-diffusion coefficients of the components with the help of the mixing rules of the Darken Due to the inconsistencies in experimental results, the dependence of diffusion on sorbate concentration is not well understood, but in general, the increase in diffusion is attributed to increase in concentration difference which is explained by Darken equation, while the decrease in diffusion is attributed to the rise in molecules collision [43, 45].

$$D_{AB}^{MD} = -2 \times 10^{-15} C^3 + 1 \times 10^{-11} C^2 - 2e^{-8}C + 3 \times 10^{-5} \qquad (7)$$

$$D_{AB}^{Calc} = -2.327 \times 10^{-10} C^3 + 1.313 \times 10^{-6} C^2 - 0.0021474C + 2.975411 \qquad (8)$$

Table 5. Molecular dynamics simulated diffusion coefficient and predicted diffusion coefficient by Eq. (10) of methane in water for various temperature and concentration.

T(k)	Concentration (ppm)	D_{AB}^{MD}(cm²/s)$\times 10^5$	D_{AB}^{Calc}(cm²/s)$\times 10^5$
298	300	2.44276	2.474
298	400	2.275016	2.283
298	500	2.246983	2.16
298	1000	1.90013	1.931
298	1500	1.92625	1.928
298	2000	2.05433	2.026
298	2500	2.196516	2.205
293	1000	1.844856	1.824
303.05	1000	1.99425	2.043
308.25	1000	2.11698	2.164
315.75	1000	2.38968	2.347
320	1000	2.452216	2.455

Table 6. Errors of molecular dynamics simulated diffusion coefficient and predicted diffusion coefficient by Eq. (10) of methane in water for various temperature and concentration.

	Calc.
R^2	96.54987
R^2_{adj}	93.67477
R_{MSD}	1.096×10^{-7}
Variance	2.885×10^{-13}

Eq. (9) was presented to predict diffusion coefficient of methane in water as a function of temperature and concentration. The obtained diffusion data from molecular dynamics simulation was adjusted by result of Eq. (9); hence, the desired coefficients were calculated by Eq. (10) as indicated in Table 5 in which result of the equation are represented. Table 6 also, shows accuracy of Eq. (10). Figure 6-a demonstrates

Figure 6. a) diffusion coefficient acquired from molecular dynamics simulation and calculated by Eq. 10b) molecular dynamics simulated diffusion coefficient versus predicted data by Eq. (10).

diffusion data at constant temperature and concentration for both case of simulated by molecular dynamics and predicted by Eq. (10). Figure 6-b illustrates the molecular dynamics simulated diffusion coefficient versus predicted diffusion coefficient by Eq. (10), in which the R^2 for fitted line in Figure 6-b is equal to 96.56% that shows high precision of Eq. (10).

$$D_{AB} = \frac{kT^n C^m + s}{C^z + x} \tag{9}$$

$$D_{AB} = \frac{8.228 \times 10^{-13} T^{3.426586} C^{-0.7410594} + 2.347 \times 10^{-8}}{C^{-0.1865813} - 0.1865813} \tag{10}$$

3. Conclusion

In this study, the diffusion coefficient of methane in water was predicted at different temperatures and concentrations. Firstly, a comparison was made between experimental and simulation results that indicated the validity of the model and the field force model. Furthermore, the effect of temperature and concentration on the methane diffusion coefficient in water was investigated. As the temperature increases with rise in molecular motion of the gas, the diffusion coefficient also enhances. The diffusion coefficient initially decreases by increasing the concentration and it reaches to a plateau at a concentration of 1000 ppm. Then, it meets an increases. In addition, the diffusion coefficient is obtained through a function of the third order concentration. Finally, in order to predict the diffusion coefficient, a function was proposed based on the concentration and temperature, which showed an agreement with simulation results by molecular dynamics.

In overall, our primary work has focused on simulation, which acts as a bridge in another sense: between theory and experiment. We could test a theory by conducting a simulation using the same model. Additionally, the models were tested by comparing with experimental data. Moreover, the simulation's findings almost indicated same results on the computer which were difficult or takes a lot of time and money to be conducted in the laboratory.

Declarations

Author contribution statement

Hojatollah Moradi: Conceived and designed the experiments; Performed the experiments.

Hossein Bahmanyar: Analyzed and interpreted the data; Wrote the paper.

Hedayat Azizpour: Conceived and designed the experiments; Analyzed and interpreted the data; Wrote the paper.

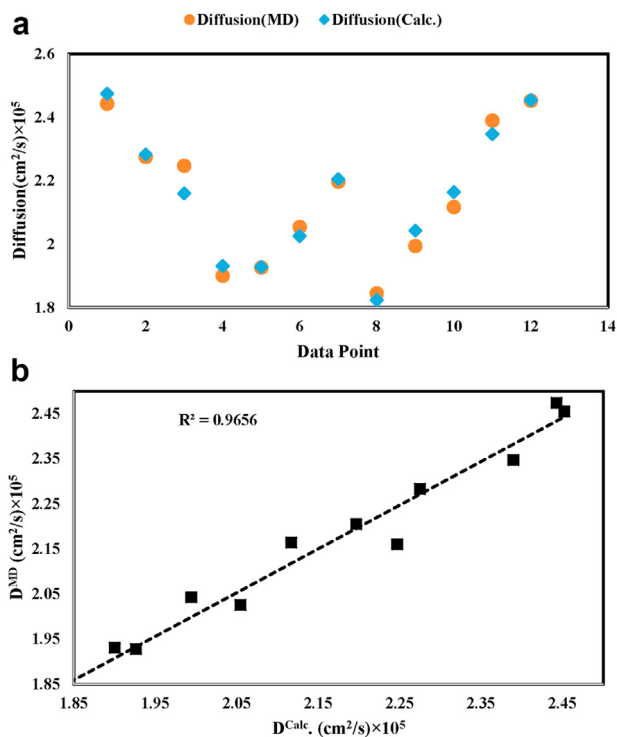Mohammad Mohammadi: Contributed reagents, materials, analysis tools or data; Wrote the paper.

Mahdi Akbari: Contributed reagents, materials, analysis tools or data.

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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