

Developing two analytical solutions for the diffusion equation and two simple mathematical models for prediction of the gas diffusivity



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ABSTRACT

The accurate prediction of the diffusion coefficient of gases in liquid hydrocarbons is of paramount importance in a variety of applications. Two general approaches are frequently employed for calculation of this property namely, empirical correlations and theory-based mathematical models. Due to lack of sound experimental data at high pressure conditions, application of empirical correlations has become limited; hence, most researchers have employed theory-based mathematical models at these conditions to provide more accurate estimates.

The Primary aim of this study is to develop two analytical solutions for the diffusion equation in order to predict the diffusion coefficient of gases in liquids. Diffusion coefficients of methane in dodecane and also in a typical Iranian crude oil are estimated using the developed analytical solution. Two mathematical models have subsequently been developed through transferring these analytical solutions into a dimensionless form, making them easier to solve. The novelties and advantages behind the current work is that the solution of this model is not a function of empirical constants, additionally, it has no parameters that need to be adjusted. One of the fascinating features of this model is that it is quite simple, straight forward, and easy to implement.

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1. Introduction

Molecular diffusion is concerned with the movement of individual molecules through a substance by virtue of their thermal energy (Treybal, 1980). Mechanism of molecular diffusion occurs due to close contact of gas and liquid phases which are not thermodynamically at equilibrium (Jamialahmadi et al., 2006). This mechanism ultimately leads to a completely uniform concentration of substance throughout a solution which may initially have not been uniform (Treybal, 1980). The mass transfer by molecular diffusion is very important in various fields of science and engineering, including chemical engineering, petroleum engineering and Biotechnology (Jamialahmadi et al., 2006).

Diffusivity of gas–liquid systems is the most important factor to determine the transfer rate of species from one phase to another. As a common application, it is necessary to predict the rate of mass transfer between gas and oil due to a diffusion process for planning

and evaluation of gas injection projects. Molecular diffusion coefficient at reservoir condition is the most important parameter required for determining the rate of mass transfer between gas and oil phases (Jamialahmadi et al., 2006; Dorao, 2012).

Diffusion coefficient, also called Diffusivity, is an important parameter indicative of the diffusion mobility. Diffusion coefficient is not only encountered in Fick's law, but also in numerous other equations of physics and chemistry (Sidiq and Amin, 2009).

For accuracy prediction of Molecular diffusion coefficient requires two important decisions: (i) to define a reliable experimental method; and (ii) to choose accurate models for data interpretation.

Experimental methods of calculating the molecular diffusion coefficient are divided into two categories, namely direct and indirect methods (Sheikha et al., 2005; Etminan et al., 2010). First method requires the composition of the liquid phase to be known. To provide an accurate model, fluid composition and its physical and thermodynamic properties have to be updated periodically, mainly owing to continuous changes in the fluid composition (Jamialahmadi et al., 2008). Conclusively, the direct methods are usually time consuming, expensive and quite sensitive to the accuracy of the experiment (Policarpo and Ribeiro, 2011). Moreover,

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the recorded laboratory data applicable to direct methods are highly scarce and rather scattered particularly at high pressure conditions. Considering the aforementioned limitations, direct methods are less suited to predict the diffusion coefficient of hydrocarbon gases in hydrocarbon liquids within wide pressure ranges (Jamialahmadi et al., 2006). In contrast, the need for analyzing the liquid phase composition is obviated using the indirect experimental data. So the Indirect experimental methods are simpler than the direct methods while having sufficiently accurate results (Policarpo and Ribeiro, 2011). The indirect experimental methods can be classified into several types, the most important of which are pressure decay and volume-time methods.

In the pressure decay (PD) method, the gas phase is injected into the liquid phase at an isothermal condition, during which the changes in gas phase pressure are recorded versus elapsed time. However, alterations in volume of the liquid phase are generally neglected and its quantity is assumed constant in this method. Finally, the diffusion coefficient is determined using the recorded pressure decay data in conjunction with an appropriate model (Renner, 1988; Zhang et al., 2000; Sheikh et al., 2006).

In the volume-time (VT) method, the gas phase is injected into the liquid phase at constant temperature and pressure, during which the volume of the liquid phase is being recorded versus elapsed time. The diffusion coefficient is then calculated using the recorded data together with an appropriate model (Jamialahmadi et al., 2006). This model takes into account the oil phase swelling so as to provide more accurate results.

To perform the PD method, it is possible to use any PVT cell but, for the VT method, the cell must possess visual windows and a cathetometer to permit volume readings. Accordingly, the PD method is preferred because of its simplicity in experimental measurements. Although the assumption of negligible oil phase swelling in the PD method has a rather slight effect on the measured diffusion coefficient at low pressures, some deviations and errors are expected to happen at moderate and high pressures (Zhang et al., 2000; Sheikh et al., 2006). Furthermore, According to Etminan et al. (2010), the mathematical models are more complicated for the PD method compared to that of the VT method due to the pressure decline occurring mostly at the interface (Etminan et al., 2010).

In this paper, two analytical solutions to the diffusion of hydrocarbon gas molecules into crude oil and dodecane will be presented, one for the semi-infinite boundary condition and the other for the finite boundary condition. The analytical solution for the finite boundary condition is evaluated using the experimental data presented in the work of Jamialahmadi et al., (2006), based on the VT method within a wide pressure range. The data is resulted from the laboratory tests done by means of an accurate, high pressure diffusion cell with a finite domain moving boundary behavior. Finally, the diffusion coefficients of methane-dodecane and methane-crude oil are determined. Furthermore, two mathematical models are developed for the semi-infinite boundary condition and the finite boundary condition through transferring these analytical solutions into a dimensionless form. The diffusion coefficient obtained from these mathematical models are then compared with those determined by the analytical solution developed for the finite boundary condition.

2. Mathematical modeling

The mathematical model, which is used to predict the gas diffusivity in this study, is obtained from the equation of continuity of solute components. The general form of continuity equation is given in Equation (1): (Jamialahmadi et al., 2006).

$$u_x \cdot \frac{\partial C}{\partial x} + u_y \cdot \frac{\partial C}{\partial y} + u_z \cdot \frac{\partial C}{\partial z} + \frac{\partial C}{\partial t} = D \cdot \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) + R_A \quad (1)$$

For a one-dimensional diffusion cell in the absence of chemical reaction and natural convection, the equation of continuity is simplified into a form represented by Equation (2). The schematic of the diffusion process is shown in Fig. 1.

$$\frac{\partial C_A}{\partial t} = D \frac{\partial^2 C_A}{\partial x^2} \quad (2)$$

The diffusion process at high pressures can also be described by Fick's second law provided that the diffusion coefficient, D , is improved by a thermodynamic factor for non-ideal mixtures as follows (Riazi, 1996):

$$D = D_a \left(1 + \frac{\partial \ln \phi_i}{\partial \ln x_i} \right) \quad (3)$$

Where ϕ_i is the Fugacity coefficient and x_i is the mole fraction of i in the liquid phase. Ignoring the above factor for the experimental data used in this paper does not introduce a significant error into our calculations (Jamialahmadi et al., 2006). The diffusion coefficient could be determined after solving the Equation (2) according to initial and boundary conditions imposed on the problem. One initial condition and two boundary conditions are needed to solve this equation. It is assumed that the solute concentration in the liquid phase is negligible at initial condition, thus the initial condition is defined as:

$$C_A = 0 \quad \text{For } t = 0 \text{ and } 0 \leq x \leq Z \quad (4)$$

According to the film theory of Whitman (1923) (Policarpo and Ribeiro, 2011), the gas and liquid phases at the interface (i.e. $x = Z$) shown in Fig. 1 are at thermodynamic equilibrium. Thus, the interfacial solute concentration remains constant as long as the pressure and temperature of the diffusion cell are kept unaltered. The first boundary condition is then defined as:

$$C_A = C_{Ai} \quad \text{For } x = Z \text{ and } t > 0 \quad (5)$$

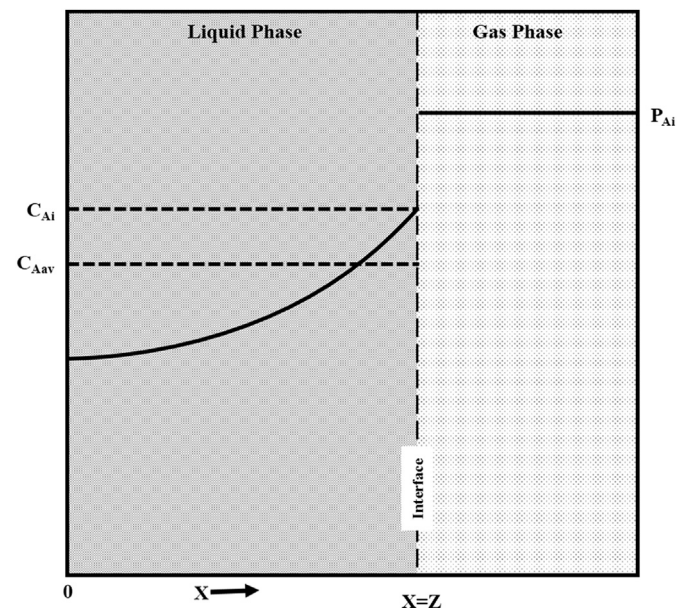


Fig. 1. One-dimensional diffusion process in a test diffusion cell.

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