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Thermodynamics of Thermal Diffusion Factors in Hydrocarbon Mixtures

Keshawa Shukla

Abstract

The reliable evaluation of thermal diffusion factors is important to understand the composition variation of the mixture components in hydrocarbon reservoirs. A thermodynamic model of thermal diffusion factors of hydrocarbon mixtures is presented. The model is based on the statistical theory of linear transport of intermolecular forces and accounts for the explicit effects of molecular mass, energy and size parameters. The accuracy of the model is first evaluated by comparing calculated results with the available non-equilibrium molecular dynamics simulation results. The theoretical model is then applied to explain thermal diffusion factors in some selected binary hydrocarbon mixtures over a range of temperature, pressure and molecular composition conditions.

Keywords: hydrocarbon mixtures, thermodynamics, thermal diffusion, molecular interaction, reservoirs

1. Introduction

This chapter deals with one of the key aspects of hydrocarbon production from the oil and gas reservoirs, known as the thermal diffusion process. This process plays an important role to separate isotopic mixtures and isobaric mixtures, analyze hydrodynamic instability in mixtures, transport mass in living matters, migrate minerals, separate and characterize polymers and colloidal particles by thermal field flow fractionation. In the case of hydrocarbon productions, the thermal diffusion process is generally used to study the compositional variation and segregation in hydrocarbon oil and gas reservoirs [1, 2].

In some hydrocarbon reservoirs, very large compositional variations can be observed in horizontal and vertical directions. There is a large temperature gradient in the vertical direction, and a small temperature gradient in the horizontal direction. The horizontal temperature gradient always induces both thermal convection and thermal diffusion, while the vertical temperature gradient causes thermal diffusion but may or may not induce thermal convection. The temperature gradient develops a concentration gradient of the mixture constituents. A thermal diffusion process takes place when the convection free gas and liquid mixture tend to separate under a temperature gradient. This phenomenon is known as the “Soret Effect.” This effect can be measured by means of thermal diffusion factor (α_T).

A significant progress has been made in recent past to measure thermal diffusion factors in liquid mixtures [3, 4].

The available experimental data have indicated that in low pressure gaseous mixtures and ideal liquid mixtures, α_T is small, and molecular size and mass govern its magnitude [5]. On the other hand, α_T may be large in non-ideal liquid mixtures where energy interactions, size and shape of the molecules, and thermodynamic conditions govern the magnitude of α_T [6]. Also, the thermal diffusion can enhance composition gradient in vertical direction in hydrocarbon reservoirs [7], and it can enhance or weaken compositional variation in vertical direction as thermal diffusion is usually opposite in sign to the gravitational segregation in hydrocarbons reservoirs [8, 9].

Therefore, a reliable theoretical model of thermal diffusion factors in hydrocarbon mixtures is required to accurately predict the compositional variations in reservoirs and evaluate the formation fluid.

There has been a continued interest in the thermodynamic modeling and the measurement of thermal diffusion factors in multicomponent mixtures (e.g., [10–16]). Numerous classical thermodynamic approaches have been utilized to describe the thermal diffusion factors in binary hydrocarbon mixtures only qualitatively [10–13]. A more successful thermodynamic model of thermal diffusion factors of non-ideal mixtures was presented by Shukla and Firoozabadi [2, 14]. The model was based on the thermodynamics of irreversible processes and kinetic theory, combining both the equilibrium and non-equilibrium properties. In this model, the equilibrium properties were determined from the equation of state while the non-equilibrium properties were obtained from the fluid viscosity. The model predictions of thermal diffusion factors in several binary mixtures were found to represent the experimental data very well. However, the signs of thermal diffusion factors of components could not establish uniquely the direction of warmer and colder region of fluids, especially in multicomponent mixtures. Furthermore, these models provide little or no information about the intermolecular forces in the system, and cannot describe adequately the thermal diffusion factors close to the critical point of the fluids.

Several attempts were made in the past to better describe thermal diffusion factors of gaseous hydrocarbon mixtures using statistical thermodynamics and molecular simulations depending on the intermolecular interactions [17–19]. A review of the developments in the theory and experiment of thermodiffusion has been presented recently by Kohler and Morozov [20]. However, the statistical theory of thermal diffusion was not applied to the liquid hydrocarbon mixtures of industrial interest. Moreover, the rigorous theories were not available to express the volumetric and heat flow properties accurately.

Recently, Shukla [21] proposed a model of thermal diffusion factors in hydrocarbon mixtures using the statistical thermodynamics of intermolecular interactions [22]. The model was able to describe the thermal diffusion factors of several binary hydrocarbon and non-hydrocarbon mixtures. The objective of this paper is to examine the accuracy of the proposed model in describing thermal diffusion factors of binary hydrocarbon mixtures.

Section 2 describes briefly the relation between the mass flux and thermal diffusion coefficient of a binary fluid mixture. Section 3 establishes the relation between statistical thermodynamics of thermal diffusion factors and how to account for the intermolecular interactions of the molecular constituents. Section 4 compares theoretical results with experimental data and examines the reliability of the theory for the selected binary hydrocarbon mixtures. Section 5 presents the conclusion of this study.

2. Thermal diffusion coefficients

We consider a binary fluid mixture. The total diffusive mass flux of component 1 of the mixture is given by [21, 23]

$$\vec{J}_1^{(t)} = -(\rho_m^2/\rho)M_1M_2D_{12}\left[\nabla x_1 + \frac{M_1x_1}{RT}\left(\frac{\bar{V}_1}{M_1} - \frac{1}{\rho}\right)\nabla P/F_1 - \kappa_T\nabla \ln T\right] \quad (1)$$

where, ρ_m is total molar density, M is molecular weight, T is temperature, x_1 is mole fraction of component 1, ρ is mass density, P is pressure, R is gas constant, \bar{V}_1 is the partial molar volume of component 1, D_{12} is molecular diffusion coefficient, κ_T is thermal diffusion ratio of component 1, ∇ is the gradient operator, and

$$F_1 = (\partial \ln f_1 / \partial \ln x_1)_{T,P} \quad (2)$$

where f_1 is the fugacity of component 1.

The first, second and third parts of Eq. (1) arise due to the molecular diffusion, pressure diffusion and thermal diffusion. The thermal diffusion factor α_T of component 1 is defined as

$$\alpha_T = \kappa_T / x_1 x_2 \quad (3)$$

For a binary mixture, the thermal diffusion factor of component 2 has the opposite sign.

Here we consider a one dimension case in steady state, and assume that there are no convection and gravity segregation. Therefore, the mass flux can be assumed to be zero. Under these conditions, the composition and the temperature gradients are related through the following equation [2]:

$$dx_1/dz = (\alpha_T x_1 x_2 d \ln T/dz) \quad (4)$$

3. Thermodynamics of thermal diffusion factor

Here we present the thermodynamic theory based on the modified form of Chapman and Cowling [22] and Kihara [24] as applied to binary hydrocarbon mixtures. This approach involves the calculation of collision integrals of the fluid mixture for a well-defined potential function. The calculation of the transport property collision integrals for gases, whose molecules obey a simple intermolecular potential, enables to explain the transport properties of slightly non-ideal gas mixtures following the isotropic intermolecular interactions. For non-ideal mixtures, in which molecules interact with strongly anisotropic intermolecular interactions, additional contributions are assumed arising from the expansion of non-equilibrium distributions. These anisotropic interactions could affect the thermal diffusion factors significantly [25].

We consider a binary mixture of components i and j . In this mixture the molecules are assumed to interact with an effective pair-wise additive intermolecular potential function (Exp-6), given by

$$u_{ij}(r) = \varepsilon_{ij} \left[\frac{\alpha_{ij}}{\alpha_{ij} - 6} \exp(\alpha_{ij}\{1 - r/r_{mij}\}) - \frac{\alpha_{ij}}{\alpha_{ij} - 6} (r_{mij}/r)^6 \right] \quad (5)$$

where u_{ij} is the potential energy of two molecules of species i and j at a separation distance r , ε_{ij} is the depth of the potential minimum which is located at r_{mij} , α_{ij} determines the softness of the repulsion energy, and k_B is the Boltzmann's constant. In this (Exp-6) potential function, the molecules of mixture species are represented by the size parameter (R_{mab}) and energy parameter (ε_{ab}/k_B).

Using the m^{th} -order Chapman-Cowling approximation, the general form of the thermal diffusion factor (α_T) can be given by

$$(\alpha_T)_m = \frac{5}{2x_1x_2A_{00}^{(m)}} \left[x_1A_{01}^{(m)} \left(\frac{M_1 + M_2}{2M_1} \right)^{0.5} + x_2A_{0-1}^{(m)} \left(\frac{M_1 + M_2}{2M_2} \right)^{0.5} \right] \quad (6)$$

where, x_1 and x_2 are the mole fractions. M_1 and M_2 are the molecular weights of the mixture components 1 and 2. $A^{(m)}$ is a determinant of $(2m + 1)$ order, whose general term is A_{ij} , where i and j range from $-m$ to $+m$, including zero. The minor of $A^{(m)}$ obtained by striking out the row and column containing A_{ij} is denoted by the symbol $A_{ij}^{(m)}$. Similarly, the i and j th minor of $A_{00}^{(m)}$ is denoted by the symbol $A_{ij00}^{(m)}$. The elements A_{ij} are functions of the mole fractions, molecular weights and collision integrals, which are functions of temperature, molecular size and energy parameters.

From Eqs. (3) and (7) the m^{th} -order thermal diffusion ratio $(k_T)_m$ can be defined as

$$(k_T)_m = x_1x_2(\alpha_T)_m \quad (7)$$

and the collision integrals are given by the following equations:

$$\Omega^{(l)}(n) = \left(\frac{k_B T}{2\pi\mu} \right)^{0.5} \int_0^\infty \exp(-\gamma^2) \gamma^{2n+3} Q^{(l)}(g) d\gamma \quad (8)$$

$$Q^{(l)}(g) = 2\pi (1 - \cos^l \chi) b db \quad (9)$$

with

$$\gamma^2 = \frac{\mu g^2}{2k_B T} \quad (10)$$

where μ is the reduced mass of a pair of colliding molecules, and g is the initial relative speed of the colliding pair. The molecules are deflected by the collision through a relative angle χ which is a function of g and the collision parameter b .

The dimensionless collision integrals of the above equations can be expressed as follows:

$$\Omega^{(l,n)*} = \left(\frac{4}{\sigma^2(1+n)!} \right)^{-1} \left(1 - \frac{1 + (-1)^l}{2(1+l)} \right)^{-1} \left(\frac{\mu}{2\pi k_B T} \right)^{0.5} \Omega^{(l)}(n) \quad (11)$$

where $\Omega^{(l,n)*}$ is the dimensionless collision integral reduced with respect to that of the diameter σ of a rigid elastic sphere.

Using the first-order approximation, Eq. (7) is written as

$$(\alpha_T)_1 = (6C_{12}^* - 5) \left[\frac{x_1 S_1 - x_2 S_2}{x_1^2 Q_1 + x_2^2 Q_2 + x_1 x_2^2 Q_{12}} \right] \quad (12)$$

where the parameters S_1 , S_2 , Q_1 and Q_2 are given by

$$S_1 = \frac{M_1}{M_2} \left(\frac{2M_2}{M_1 + M_2} \right)^{0.5} \left(\frac{\Omega_{11}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\sigma_{11}}{\sigma_{12}} \right)^2 - \frac{4M_1M_2A_{12}^*}{(M_1 + M_2)^2} - \frac{15M_2(M_2 - M_1)}{2(M_1 + M_2)^2} \quad (13)$$

$$S_2 = \frac{M_2}{M_1} \left(\frac{2M_1}{M_1 + M_2} \right)^{0.5} \left(\frac{\Omega_{22}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\sigma_{22}}{\sigma_{12}} \right)^2 - \frac{4M_1M_2A_{12}^*}{(M_1 + M_2)^2} - \frac{15M_1(M_1 - M_2)}{2(M_1 + M_2)^2} \quad (14)$$

$$Q_1 = \left(\frac{2}{M_2(M_1 + M_2)} \right) \left(\frac{2M_2}{(M_1 + M_2)} \right)^{0.5} \left(\frac{\Omega_{11}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\sigma_{11}}{\sigma_{12}} \right)^2 \left[\left(\frac{5}{2} - \frac{6}{5}B_{12}^* \right) M_1^2 + 3M_2^2 + \frac{8}{5}M_1M_2A_{12}^* \right] \quad (15)$$

$$Q_2 = \left(\frac{2}{M_1(M_1 + M_2)} \right) \left(\frac{2M_1}{(M_1 + M_2)} \right)^{0.5} \left(\frac{\Omega_{22}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\sigma_{22}}{\sigma_{12}} \right)^2 \left[\left(\frac{5}{2} - \frac{6}{5}B_{12}^* \right) M_2^2 + 3M_1^2 + \frac{8}{5}M_1M_2A_{12}^* \right] \quad (16)$$

$$Q_{12} = 15 \left(\frac{M_1 - M_2}{M_1 + M_2} \right)^2 \left(\frac{5}{2} - \frac{6}{5}B_{12}^* \right) + \left(\frac{4M_1M_2A_{12}^*}{(M_1 + M_2)^2} \right) \left(11 - \frac{12}{5}B_{12}^* \right) + \frac{8(M_1 + M_2)}{5(M_1M_2)^{0.5}} \left(\frac{\Omega_{11}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\Omega_{22}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \left(\frac{\sigma_{11}}{\sigma_{12}} \right)^2 \left(\frac{\sigma_{22}}{\sigma_{12}} \right)^2 \quad (17)$$

A_{12}^* , B_{12}^* and C_{12}^* are functions of the collision integrals as given by

$$A_{12}^* = \left(\frac{\Omega_{12}^{(2,2)*}}{\Omega_{12}^{(1,1)*}} \right) \quad (18)$$

$$B_{12}^* = \left(\frac{5\Omega_{12}^{(1,2)*} - 4\Omega_{12}^{(1,3)*}}{\Omega_{12}^{(1,1)*}} \right) \quad (19)$$

$$C_{12}^* = \left(\frac{\Omega_{12}^{(1,2)*}}{\Omega_{12}^{(1,1)*}} \right) \quad (20)$$

The details on the various parameters are given elsewhere [21].

To consider the effects of pressure and unlike interaction parameters, Eq. (21) for C_{12}^* was modified empirically as follows:

$$C_{12}^* = \left(\frac{\Omega_{12}^{(1,2)*}}{\Omega_{12}^{(1,1)*}} \right) [\exp(p_1^*f_1 + p_2^*f_2 + p_3^*f_3)] \quad (21)$$

where p_i are the mixture parameters and f_i terms are given by

$$\begin{aligned} f_1 &= x_1 P_x^* / T_x^* \\ f_2 &= f_1^2 \\ f_3 &= f_1^3 \end{aligned} \quad (22)$$

where the reduced pressure and temperature are given in terms of energy and size parameters of the molecules

$$\begin{aligned} P_x^* &= PR_{mx}^3/\varepsilon_x \\ T_x^* &= kT/\varepsilon_x \end{aligned} \tag{23}$$

The following van der Waals mixing rules were applied to determine the mixture properties:

$$R_{mx}^3 = \sum_{i,j=1}^2 x_i x_j R_{mij}^3 \tag{24}$$

$$\varepsilon_x R_{mx}^3 = \sum_{i,j=1}^2 x_i x_j \varepsilon_{ij} R_{mij}^3 \tag{25}$$

$$R_{mij} = (R_{mii} + R_{mjj})/2 \tag{26}$$

$$\varepsilon_{ij} = (\varepsilon_{ii} \varepsilon_{jj})^{0.5} \tag{27}$$

Since the properties of the reservoir fluids depend on the fluid compositions, temperature and pressure, and since the collision integrals do not account for the pressure effects of the liquid mixtures, the empirical Eq. (22) was applied to explain the properties of the reservoir fluid mixtures under both temperature and pressure as needed.

4. Results and discussion

In this section, the performance of the thermodynamic theory is examined to represent the thermal diffusion factors in a few selected binary gas and liquid mixtures.

4.1 Potential parameters

The intermolecular potential parameters along with molecular weight of the pure fluids involved in binary mixtures studied in this work are given in **Table 1**. Molecular parameters (ε/k_B , R_m and α) are based on the correlation of the pure fluid viscosity and/or second virial coefficient data at the ambient pressure [25]. The unlike interaction parameters (R_{mij} , ε_{ij}) were evaluated following the arithmetic rule for R_{mij} and geometric rule for ε_{ij} . α was kept the same for all the fluids. The

Fluid	$\varepsilon/k, K$	R_m, A°	α	M
C ₁	148.20	3.850	14	16
C ₃	281.86	5.331	14	44
C ₄	339.35	5.755	14	58
C ₅	374.78	6.102	14	72.15
C ₇	431.13	6.861	14	100
C ₁₀	492.89	7.667	14	142.29
C ₁₆	575.42	8.827	14	226

Table 1.
(Exp-6) Potential parameters for the mixture components.

Mixture	P ₁	P ₂	P ₃
C ₁ + C ₃	−51.9	820.6	−2742.7
C ₁ + C ₄	13.2	1.34	−183.7
C ₅ + C ₁₀	−0.6864	0	0
C ₇ + C ₁₆	525.8	−21375.0	294494.2

Table 2.
Polynomial parameters of $C^*(1,2)$.

pressure and potential parameters dependences of the unlike collision integrals are expressed in terms of a simple polynomial as given in Eq. (22) above. The polynomial parameters p_i for the specific mixtures are given in **Table 2**. In this work, no effort was made to optimize the unlike energy, size and α parameters.

4.2 Application of theory to liquid mixtures of hydrocarbons

In order to check the reliability of the thermodynamic model, theoretical results are first tested against the non-equilibrium molecular dynamics simulation results using the same (Exp-6) intermolecular potential function for a binary mixture of pentane and decane (C₅ + C₁₀) [26]. Note that the optimized parameters were used in the non-equilibrium molecular dynamics simulations to represent the experimental data of thermal diffusion factors of (C₅ + C₁₀) mixture.

Figure 1 compares the theoretical results with the simulation results of α_T for the mixture of pentane and decane (C₅ + C₁₀) at 300 K and 0.1 MPa [26]. These results show that the thermodynamic model can describe α_T reasonably well with the uncertainties of simulation results. Also included in the **Figure 1** are measured data for the system (C₅ + C₁₀). The model is seen to compare well with both simulation and measured results within their data uncertainties.

The above results suggest that the thermodynamic model with the pressure dependent collision integrals offers reliable prediction of α_T as a function of both temperature and concentration in binary mixtures. Therefore, we adopted the unlike potential parameter and pressure dependent collision integrals to first

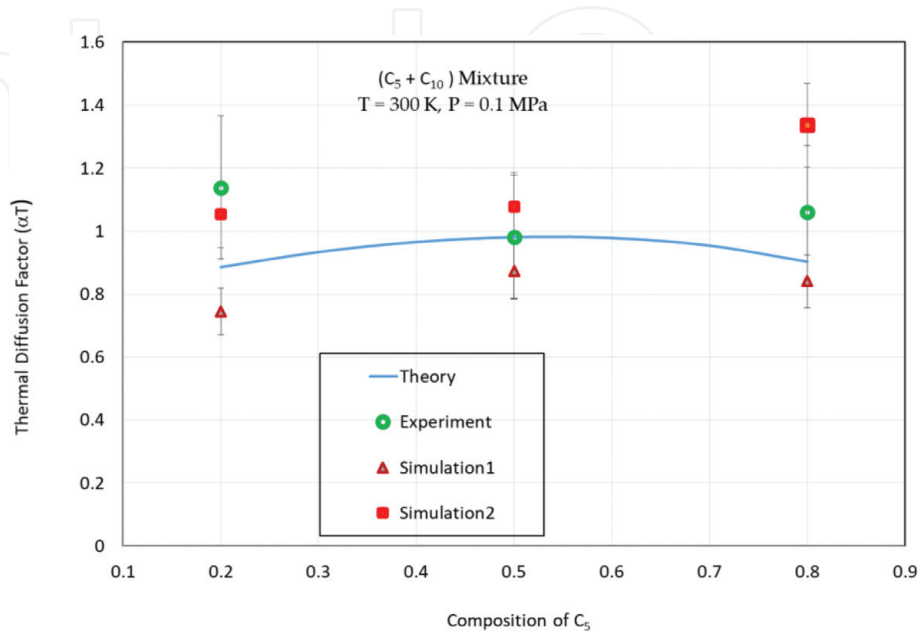


Figure 1.
Thermal diffusion factor for mixture (C₅ + C₁₀) from theory, simulation and experiment.

correlate a value of α_T in liquid hydrocarbon mixtures at a single temperature and equimolar condition, and extended that to all other conditions. When several data points of thermal diffusion factor were available in different non-ideal conditions of temperature, pressure and concentration, we re-evaluated the single point parameters by incorporating several data points in parameters regression. Also, in most of the cases the three parameters p_1 , p_2 and p_3 can describe well the diffusion factors and can depend on the temperature, pressure, concentration and interaction parameters.

Figure 2 presents results for the collision integrals independent of pressure. The calculated collision integral results are physically consistent and agree with the literature data very well [25].

Figure 3 shows theoretical predictions and experimental data [27] of α_T for mixture ($C_1 + C_3$) at a given temperature $T = 346\text{ K}$ and $P = 5.5\text{ Mpa}$ as a function of composition of C_1 . **Figure 4** presents theoretical and experimental results of α_T for $T = 346\text{ K}$, and composition, $x_1(C_1) = 0.34$ as the function of pressure. The latter

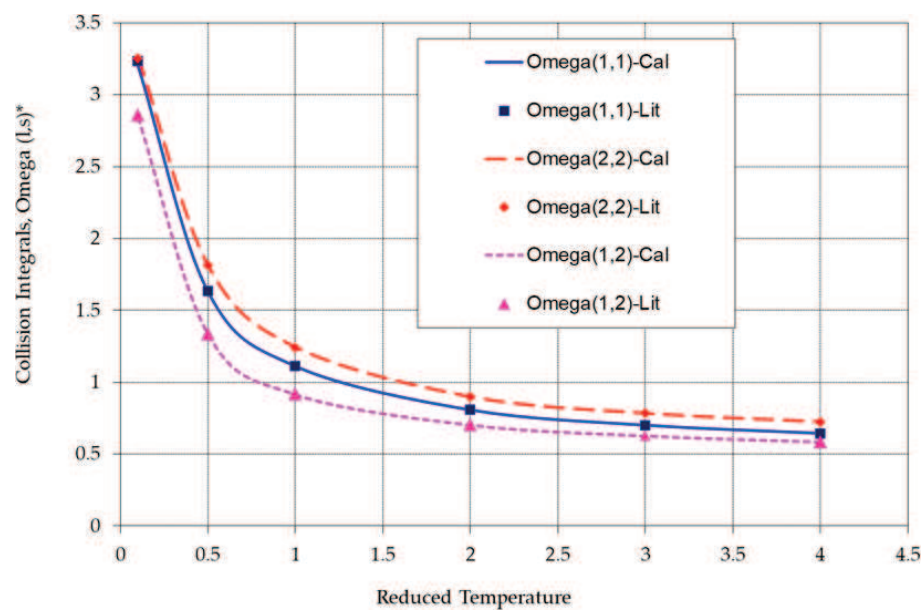


Figure 2.
Collision integrals from calculation and literature.

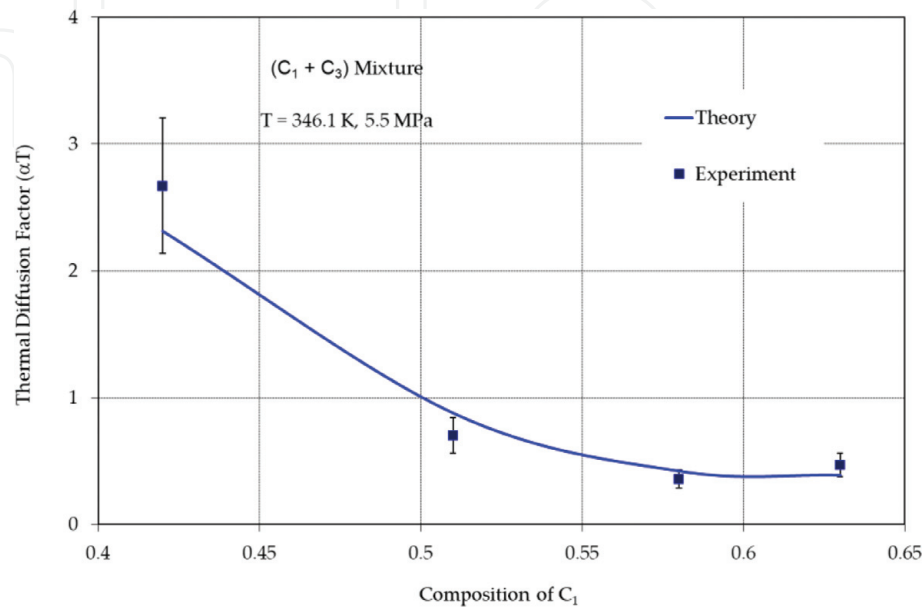


Figure 3.
Thermal diffusion factor for mixture ($C_1 + C_3$) from theory and experiment.

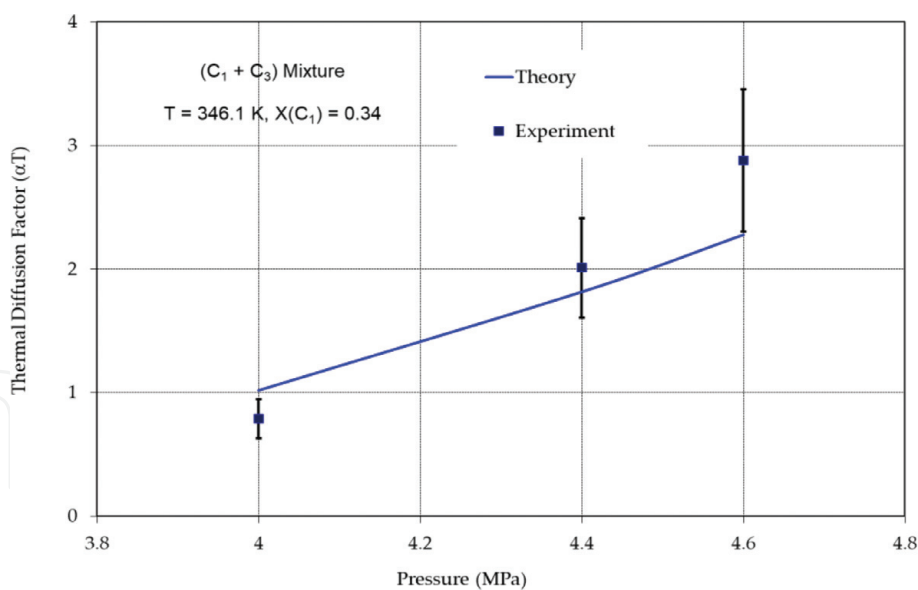


Figure 4.
Thermal diffusion factor for mixture $(C_1 + C_3)$ from theory and experiment.

condition is close to the critical point of the mixture $(C_1 + C_3)$. In both cases the theoretical results are in agreement with the measured data well within the experimental uncertainty.

Figure 5 compares theoretical predictions with experimental data [23] of α_T for mixture of methane and butane $(C_1 + C_4)$ for temperature 346 K and composition $x_1(C_1) = 0.34$. **Figure 6** presents similar comparisons at the lower temperature of 319 K and composition of $x_1(C_1) = 0.49$. The variations of thermal diffusion coefficients with pressure are investigated. The comparison between theory and experiment is very good for all the tested conditions.

To further examine the reliability of our models, **Figure 7** compares theoretical and experimental results of α_T for the more non-ideal mixture of Heptane and Hexadecane $(C_7 + C_{16})$ [28]. The model can describe α_T reasonably well over the whole range of the composition.

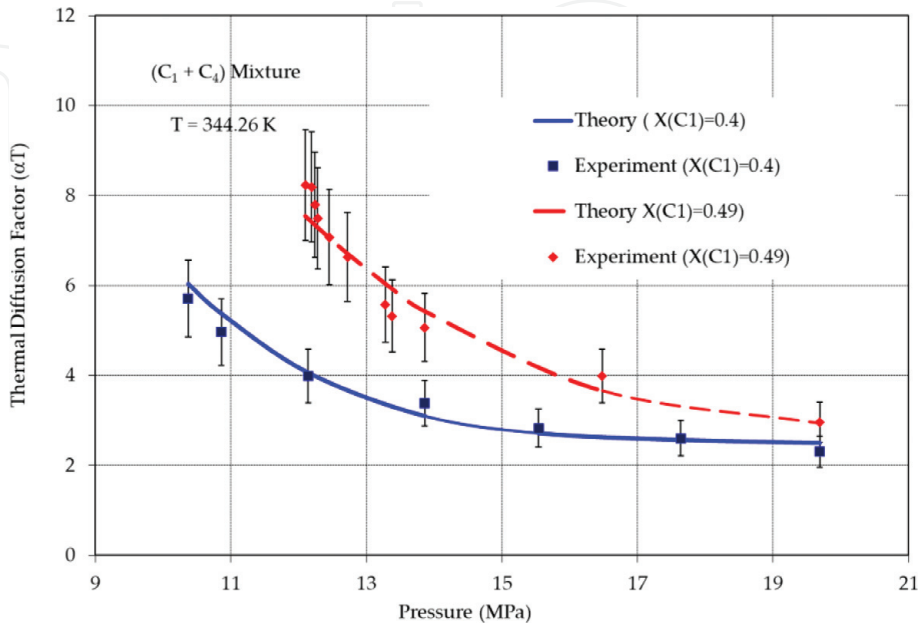


Figure 5.
Thermal diffusion factor for mixture $(C_1 + C_4)$ from theory and experiment.

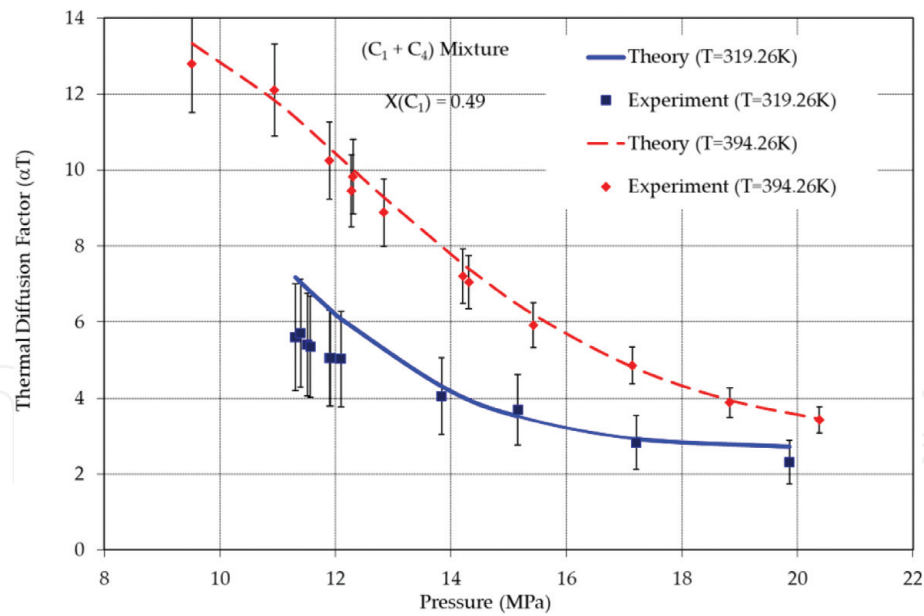


Figure 6.
Thermal diffusion factor for mixture (C₁ + C₄) from theory and experiment.

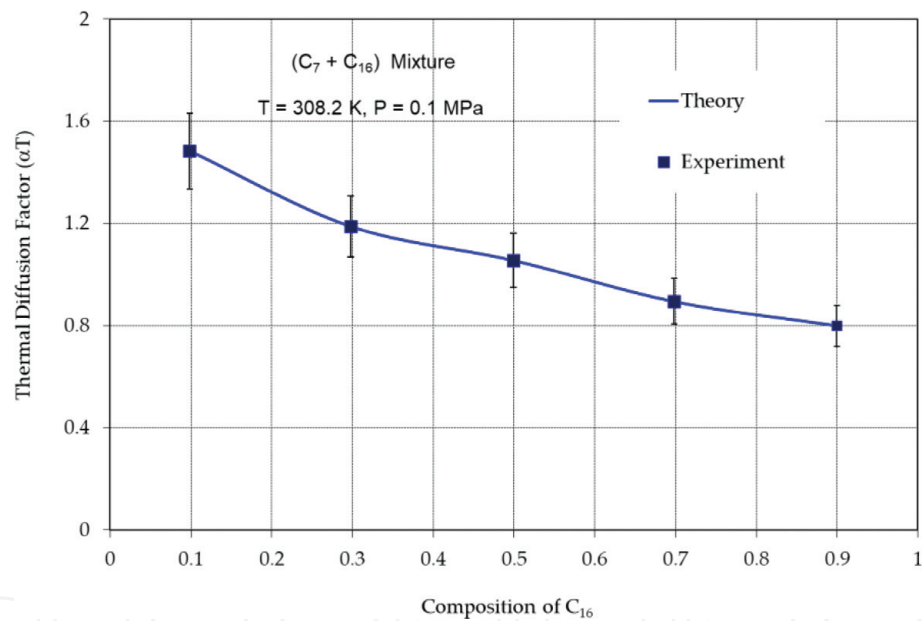


Figure 7.
Thermal diffusion factor for mixture (C₇ + C₁₆) from theory and experiment.

5. Conclusions

In this paper the statistical thermodynamics has been applied to predict the thermal diffusion factors of binary hydrocarbon systems using the thermodynamic model based on the statistical thermodynamics and the (Exp-6) potential function of two-body molecular interactions. The collision integrals were redefined to account for the energy and size parameters of the molecules in addition to their pressure and temperature dependency. Theoretical results are tested against the molecular simulation results and experimental data for a few selected binary hydrocarbon gas and liquid mixtures. The model can successfully describe the simulation results of the binary hydrocarbon mixture investigate her. In general, the comparisons of theoretical results with experimental data for the thermal diffusion

coefficients show a very good performance of the theory in different non-ideal reservoir conditions over a range of temperature, pressure and concentration. The unlike interaction parameters are seen to be important for accounting the non-ideal effects in collision integrals, and for improving the correlation and prediction of thermal diffusion factors in non-ideal hydrocarbon liquid mixtures.

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Conflict of interest


No potential conflict of interest.

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