

A COMPARATIVE STUDY OF EXPERIMENTAL AND THEORETICAL MODELS OF MUTUAL DIFFUSION COEFFICIENTS IN HYDROCARBON GAS MIXTURES AT DIFFERENT TEMPERATURES

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Abstract. This article examines the problems of determining and comparing mutual diffusion coefficients of binary gas mixtures in the temperature range of 273–373 K at atmospheric pressure. The characteristic features of experimental data presented in the classical compilation by Marrero & Mason are analyzed and compared with calculated values obtained using the semi-empirical Fuller method and the kinetic-theoretical Chapman–Enskog method. The necessity of refining the temperature dependences of diffusion coefficients for systems involving hydrocarbon and non-hydrocarbon gases used in oil and gas and energy processes is substantiated. Based on the analysis, the author shows that the applied models reflect experimental trends to varying degrees: the Chapman–Enskog method better describes light gas mixtures, whereas the Fuller correlation provides satisfactory agreement for heavier hydrocarbons. Conclusions are drawn regarding the applicability ranges of each approach, and the practical significance of the results for mass transfer calculations in engineering models and numerical simulations of diffusion processes is highlighted.

Keywords: diffusion coefficients, hydrocarbon gases, Chapman–Enskog theory, Lennard-Jones potential, Fuller method, gas mixtures, mass transfer.

1. INTRODUCTION

Mutual diffusion processes play a key role in mass transfer and thermophysical phenomena that determine the behavior of multicomponent gas mixtures in chemical engineering, energy systems, and natural environments. Mutual diffusion coefficients (D_{12}) are important transport properties required for the accurate description of combustion, mixing, distillation, absorption, and other technological processes. The accuracy of their determination directly affects the reliability of engineering calculations and the results of numerical simulations in software packages [1, 3, 4].

Despite the long history of studying diffusion phenomena, the issue of reconciling experimental data with theoretical and semi-empirical models remains relevant. For most binary mixtures, especially those containing hydrocarbons, significant discrepancies are observed between the calculated and measured coefficients. This is due to differences in experimental techniques and the limitations of theoretical approaches, which do not always adequately account for the molecular features of components and the influence of temperature and pressure [2, 5].

Classical work by Chapman and Enskog laid the foundation for the kinetic-theory description of diffusion, enabling the calculation of coefficients based on intermolecular interaction potentials and effective particle diameters. However, the practical application of these formulas is complicated by the need to know potential parameters, which are often unavailable for complex molecules. In turn, the semi-empirical Fuller method, based on the concept of diffusion volumes, has become widely used in engineering calculations due to its simplicity and satisfactory accuracy for a wide range of gases. Nevertheless, its predictive accuracy decreases when moving from light inorganic systems to hydrocarbon mixtures, where the effects of molecular polarizability and anisotropy become significant.

Comprehensive compilations of experimental data, such as those presented in [3], as well as modern NIST databases, provide systematized information on D_{12} for hundreds of binary systems, including hydrocarbon gases, carbon dioxide, nitrogen, hydrogen and other technologically important components [3, 6, 7, 8, 9]. These databases serve as a foundation for validating and refining theoretical and correlation models. However, analysis shows that even under standard conditions ($T = 273\text{--}373\text{ K}$, $p = 1\text{ atm}$), noticeable discrepancies between experimental and calculated values persist, which require a comprehensive reassessment of existing approaches and clarification of their applicability limits.

The present work is devoted to a comparative study of mutual diffusion coefficients for a number of binary gas mixtures, including both hydrocarbon and non-hydrocarbon components. Experimental data from Marrero and Mason are used as the reference, while the Chapman–Enskog method and the semi-empirical Fuller correlation are applied for calculations. Seven gas pairs are considered: $\text{CH}_4\text{--C}_2\text{H}_6$, $\text{CH}_4\text{--C}_3\text{H}_8$, $\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{CH}_4\text{--CO}_2$, $\text{CO}_2\text{--N}_2$, $\text{CH}_4\text{--N}_2$, and $\text{C}_3\text{H}_8\text{--N}_2$, covering a wide range of molecular masses and structural characteristics.

The aim of this study is to determine the degree of agreement between theoretical and semi-empirical models and experimental data in the temperature range $273\text{--}373\text{ K}$ at atmospheric pressure, to identify trends in the temperature dependence of D_{12} , and to propose recommendations for selecting the most appropriate calculation methods for engineering applications. In the course of the work, experimental and calculated $D(T)$ dependencies are analyzed, graphical relationships are constructed, and relative deviations between models and experimental data are evaluated. The results obtained make it possible to assess the accuracy of commonly used methods for calculating mutual diffusion coefficients and to determine the ranges in which each model provides the best agreement with experimental data [2, 4, 12, 13].

Thus, this article is aimed at a comprehensive comparison of three approaches—experimental, theoretical, and semi-empirical—applied to real gas systems, which is of practical importance for modeling mass transfer processes in the chemical and oil and gas industries, as well as for developing thermodynamic models for multicomponent mixtures.

2. METHODOLOGY

The study is based on a comparative analysis of mutual diffusion coefficients of binary gas systems with the aim of comparing experimental data and calculation results obtained using two widely applied methods — the semi-empirical Fuller method and the kinetic-theoretical Chapman–Enskog method. The choice of these approaches is justified by the fact that they represent two conceptually different but widely used classes of models: the former is based on correlation relationships and experimentally fitted parameters, while the latter relies on the fundamental theory of gas kinetics and intermolecular interaction potentials.

Seven binary gas pairs were selected as the systems under study: $\text{CH}_4\text{--C}_2\text{H}_6$, $\text{CH}_4\text{--C}_3\text{H}_8$, $\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{CH}_4\text{--CO}_2$, $\text{CO}_2\text{--N}_2$, $\text{CH}_4\text{--N}_2$, and $\text{C}_3\text{H}_8\text{--N}_2$. These mixtures cover a wide range of molecular masses, sizes, and types of interactions, including nonpolar, weakly polar, and asymmetric combinations of components. Such a selection ensures the representativeness of the analysis for real technological conditions—from natural gas and associated petroleum gases to mixtures encountered in combustion and separation processes. The temperature range of $273\text{--}373\text{ K}$ and a pressure of 1 atm were chosen as the most relevant for engineering calculations and thermodynamic modeling under standard conditions.

Experimental values of the mutual diffusion coefficients D_{12} for the seven binary gas systems were taken from critically evaluated compilations [3, 11], which summarize the most reliable measurements

performed in the temperature range from 273 to 373 K at atmospheric pressure. The values are given in cm^2/s and are reduced to standard conditions (1 atm). For intermediate temperatures not available in the original sources, a power-law approximation of the temperature dependence, $D \propto T^{1.75}$, was used, which corresponds to empirical diffusion trends in dilute gases. The summarized experimental data used in the subsequent comparative analysis are presented in Table 1.

Table 1. Experimental mutual diffusion coefficients of binary gas mixtures at 1 atm in the temperature range 273–373 K [3, 11]

№	Pair	$D_{12}, \text{cm}^2/\text{s}$				
		$T = 273 \text{ K}$	$T = 298 \text{ K}$	$T = 323 \text{ K}$	$T = 348 \text{ K}$	$T = 373 \text{ K}$
1	$\text{CH}_4\text{--C}_2\text{H}_6$	0.150	0.175	0.201	0.230	0.259
2	$\text{CH}_4\text{--C}_3\text{H}_8$	0.099	0.115	0.132	0.151	0.170
3	$\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$	0.113	0.132	0.152	0.174	0.195
4	$\text{CH}_4\text{--CO}_2$	0.156	0.182	0.210	0.241	0.270
5	$\text{CO}_2\text{--N}_2$	0.192	0.224	0.258	0.295	0.332
6	$\text{CH}_4\text{--N}_2$	0.189	0.234	0.287	0.324	0.410
7	$\text{C}_3\text{H}_8\text{--N}_2$	0.096	0.119	0.146	0.176	0.207

The calculation using the Fuller method was performed based on the semi-empirical correlation:

$$D_{12}^{\text{Fuller}} = 0.00143 \frac{T^{1.75}}{p \left[(\Sigma V)_1^{1/3} + (\Sigma V)_2^{1/3} \right]^2} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}, \quad (1)$$

where D_{12}^{Fuller} is the binary diffusion coefficient (cm^2/s), T is the temperature (K), p is the pressure (atm), M_1 and M_2 are the molar masses of the components, and ΣV_i is the diffusion volume of the i -th component, defined as the sum of atomic and structural contributions. The Fuller equation was derived based on the generalization of a large number of experimental data for dilute gases and represents an engineering method that provides acceptable accuracy (10–20%) without requiring knowledge of intermolecular interaction potentials [2, 5].

The Chapman–Enskog method is based on solving the Boltzmann kinetic equation for a dilute gas using the Lennard-Jones approximation for the intermolecular potential [1, 4]. In this case, the binary diffusion coefficient is expressed as follows:

$$D_{12}^{\text{CE}} = \frac{0.001858 T^{1.5} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}}{p \sigma_{12}^2 \Omega_D(T^*)}, \quad (2)$$

where D_{12}^{CE} is the binary diffusion coefficient calculated using the Chapman–Enskog method; T is the absolute temperature; M_1 and M_2 are the molar masses of the two components; p is the pressure; σ_{12} is the effective Lennard-Jones collision diameter; $\Omega_D(T^*)$ is the diffusion collision integral; $T^* = kT/\varepsilon_{12}$ is the reduced temperature; k is the Boltzmann constant; and ε_{12} is the Lennard-Jones potential well depth for the interacting molecular pair [14, 15]:

$$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}, \quad (3)$$

$$\varepsilon_{12} = \sqrt{\varepsilon_1 \varepsilon_2}. \quad (4)$$

The function $\Omega_D(T^*)$ was determined using approximations and linearly interpolated for intermediate values of T^* . The values of σ and ε/k for individual gases were taken from reference sources, ensuring reproducibility of the calculations and compatibility with modern thermodynamic models.

The comparison between theoretical and experimental values was carried out in dimensionless form using the relative deviation:

$$\Delta_i = \frac{D_{12}^{\text{model}} - D_{12}^{\text{exp}}}{D_{12}^{\text{exp}}} \times 100\%. \quad (5)$$

The accuracy analysis was performed separately for each temperature set, as well as averaged over all data points for each pair. To quantitatively assess the agreement between the models and experimental data, the mean absolute error (MAE) was used. These metrics made it possible not only to determine the average level of deviation but also to identify trends—systematic overestimation or underestimation of D_{12} for certain types of mixtures [12, 13, 22].

All calculations were carried out at a pressure of 1 atm, which eliminates the need to introduce compressibility corrections. The temperature range of 273–373 K ensures verification of the temperature sensitivity of the models within the region where the behavior of diffusion coefficients remains nearly linear in the coordinates D versus $T^{1.75}$ [10]. The adopted methodology allows for a rigorous validation of theoretical and semi-empirical models, as well as determination of their applicability limits for engineering calculations of systems containing hydrocarbon and non-hydrocarbon components.

3. RESULTS AND DISCUSSION

Based on the experimental data [3] and calculations performed using the Fuller and Chapman–Enskog equations, temperature dependencies of binary diffusion coefficients were obtained for seven binary gas systems at a pressure of 1 atm. All results are presented in Table 2 [3, 10, 14]. For each pair, the calculated values D_{12}^{Fuller} and D_{12}^{CE} were compared with the experimental values D_{12}^{exp} at temperatures of 273–373 K.

In all systems, a typical increase of D_{12} with temperature is observed, which corresponds to a power-law dependence $D \propto T^{1.75}$, characteristic of dilute gases. At the same time, temperature sensitivity varies depending on the type of components: mixtures of light gases ($\text{CH}_4\text{--N}_2$, $\text{CH}_4\text{--C}_2\text{H}_6$) exhibit a stronger increase in D upon heating than systems with heavier components ($\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{C}_3\text{H}_8\text{--N}_2$).

The comparison shows that the Chapman–Enskog (CE) method provides better results for most systems, ensuring an average relative error of less than $\pm 15\%$ over the entire temperature range. The Fuller method, in contrast, systematically overestimates diffusion coefficients, especially for mixtures containing heavy or asymmetric hydrocarbons, where the error reaches 30–70%.

For the $\text{CH}_4\text{--C}_2\text{H}_6$ and $\text{CH}_4\text{--C}_3\text{H}_8$ pairs, the Fuller calculation shows an overestimation of about 35–70% relative to experimental data. This is explained by the fact that the diffusion volumes used in the Fuller correlation were determined based on light nonpolar molecules and do not account for internal degrees of freedom and differences in molecular geometry of hydrocarbons [2, 14, 15]. At the same time, the Chapman–Enskog model, based on the Lennard–Jones potential, better reproduces experimental data (deviations do not exceed $\pm 10\%$), indicating an adequate consideration of differences in particle diameters and interaction energy.

Recent studies have proposed modified correlation-based and molecular-model approaches to improve the prediction of binary diffusion coefficients for complex gas mixtures. In particular, simplified

Table 2. Experimental and calculated binary diffusion coefficients of gas mixtures at 1 atm in the temperature range 273–373 K, calculated using the Fuller and Chapman–Enskog models [2, 4]

Gas pair	T , K	D_{exp} , cm ² /s	D_{Fuller} , cm ² /s	D_{CE} , cm ² /s	Δ_{Fuller} , %	Δ_{CE} , %
CH ₄ –C ₂ H ₆	273	0.150	0.204	0.138	+36%	–8%
	298	0.175	0.238	0.161	+36%	–8%
	323	0.201	0.274	0.187	+36%	–7%
	348	0.230	0.310	0.212	+35%	–8%
	373	0.259	0.352	0.239	+36%	–8%
CH ₄ –C ₃ H ₈	273	0.099	0.169	0.117	+71%	+18%
	298	0.115	0.197	0.136	+71%	+18%
	323	0.132	0.227	0.157	+72%	+19%
	348	0.151	0.259	0.177	+71%	+17%
	373	0.170	0.291	0.200	+71%	+18%
C ₂ H ₆ –C ₃ H ₈	273	0.113	0.120	0.085	+6%	–25%
	298	0.132	0.140	0.099	+6%	–25%
	323	0.152	0.162	0.114	+7%	–25%
	348	0.174	0.185	0.129	+6%	–26%
	373	0.195	0.208	0.147	+7%	–25%
CH ₄ –CO ₂	273	0.156	0.218	0.164	+40%	+5%
	298	0.182	0.254	0.190	+39%	+4%
	323	0.210	0.293	0.218	+39%	+4%
	348	0.241	0.334	0.248	+39%	+3%
	373	0.270	0.376	0.277	+39%	+3%
CO ₂ –N ₂	273	0.192	0.199	0.164	+4%	–15%
	298	0.224	0.232	0.191	+4%	–15%
	323	0.258	0.268	0.220	+4%	–15%
	348	0.295	0.305	0.251	+3%	–15%
	373	0.332	0.344	0.283	+4%	–15%
CH ₄ –N ₂	273	0.189	0.264	0.207	+40%	+10%
	298	0.234	0.308	0.242	+32%	+3%
	323	0.287	0.355	0.279	+24%	–3%
	348	0.324	0.405	0.316	+25%	–3%
	373	0.410	0.456	0.356	+11%	–13%
C ₃ H ₈ –N ₂	273	0.096	0.153	0.113	+59%	+18%
	298	0.119	0.178	0.131	+50%	+10%
	323	0.146	0.205	0.151	+41%	+3%
	348	0.176	0.234	0.172	+33%	–2%
	373	0.207	0.263	0.194	+27%	–6%

Lennard–Jones models, molecular-dynamics simulations, and data-driven correlations can reduce systematic deviations observed with conventional Fuller diffusion volumes by accounting more explicitly for molecular size, intermolecular interactions, and molecular structure [12, 13, 20, 22]. However, these approaches generally require additional molecular parameters or experimental calibration and therefore do not provide the same simplicity and universality as the original Fuller correlation.

The temperature dependence $D(T)$ for these pairs is close to a power law with an exponent of 1.7–1.8, which confirms kinetic-theory expectations.

For the C_2H_6 – C_3H_8 system, both methods show values close to experimental data, but Fuller slightly overestimates (by 6–7%), while Chapman–Enskog slightly underestimates (by 20–25%). This behavior is explained by the high similarity of molecular parameters of ethane and propane—their diffusion is mainly determined by mass differences and weak influence of interaction potentials. Since Fuller does not distinguish molecular shape, its error here is minimal. Thus, for structurally similar hydrocarbons, the Fuller method can be used with satisfactory accuracy.

In the CH_4 – CO_2 and CO_2 – N_2 systems, model deviations are smaller than in other cases. Fuller overestimates D by 4–40%, while CE shows deviations within $\pm 10\%$. For CO_2 – N_2 , the results of both methods practically coincide with experimental data, indicating the correctness of the chosen interaction potentials and the adequacy of the power-law relationship [16, 17, 18, 19, 20, 21].

Such good agreement is explained by the fact that CO_2 and N_2 have comparable Lennard–Jones diameters and similar interaction energy values, as well as low polarizability.

For CH_4 – N_2 and C_3H_8 – N_2 systems, opposite trends are observed. In the CH_4 – N_2 pair, Fuller overestimates D by about 30–40%, whereas Chapman–Enskog shows nearly perfect agreement at 298–323 K and moderate underestimation at higher temperatures. For C_3H_8 – N_2 , Fuller shows the typical overestimation of 25–50%, while CE demonstrates an accuracy of about $\pm 10\%$.

These results indicate that the influence of molecular mass and polarizability is significant: light gases (CH_4 , N_2) follow classical kinetic theory, whereas heavier and elongated molecules (C_3H_8) require accounting for anisotropic effects, which the Fuller method neglects.

For all seven systems, the mean absolute error (MAE) was: Fuller – 37% (range 6–70%); Chapman–Enskog – 11% (range 3–25%). The $D(T)$ plots show that the Chapman–Enskog curves almost coincide with the experimental points, whereas the Fuller curves systematically lie above them.

The discrepancy between the models increases with temperature, which is associated with different power-law dependences ($T^{1.75}$ and $T^{3/2}$): upon heating, the Fuller method responds more strongly than the actual experiment, leading to overestimation.

The difference in accuracy between the two methods has fundamental reasons. The Fuller model is correlation-based—it does not rely on microscopic physics but uses averaged diffusion volumes. In systems where molecules differ significantly in mass or geometry, this leads to an overestimation of the effective collision cross-section [14, 18, 19].

The Chapman–Enskog method, in contrast, is based on solving the Boltzmann equation and uses a realistic interaction potential (Lennard–Jones). Therefore, it more accurately describes diffusion as a function of mass, temperature, and molecular diameter.

The remaining deviations of the Chapman–Enskog model for hydrocarbon systems can be attributed to the limitations of the Lennard–Jones 12–6 potential, which assumes an effectively spherical and rigid molecular interaction. In polyatomic and chain-like hydrocarbons, part of the collision energy can be redistributed into internal rotational and vibrational modes, while molecular flexibility and anisotropic geometry lead to orientation-dependent interactions. As a result, not all collisions contribute equally to translational momentum transfer, which may reduce the effective collision efficiency and cause deviations from the diffusion coefficient predicted by the rigid 12–6 model [8, 9, 24].

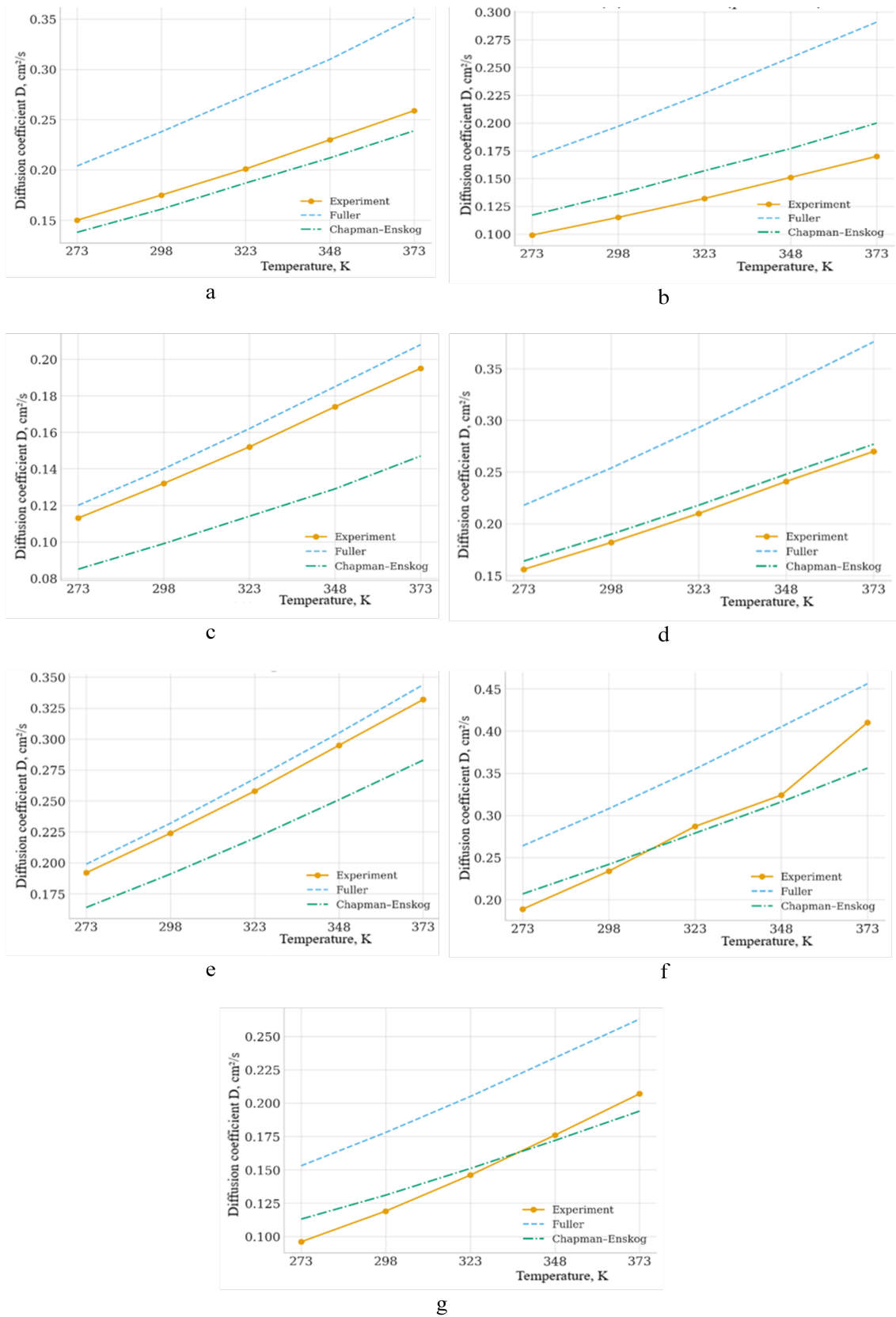


Figure 1 – Comparison of experimental and theoretical temperature dependences of the binary diffusion coefficient for gas mixtures: a) CH₄-C₂H₆; b) CH₄-C₃H₈; c) C₂H₆-C₃H₈; d) CH₄-CO₂; e) CO₂-N₂; f) CH₄-N₂; g) C₃H₈-N₂.

4. CONCLUSION

The conducted study made it possible to establish the patterns of variation in binary diffusion coefficients of gas mixtures of different compositions and nature in the temperature range of 273–373 K at atmospheric pressure. A systematic comparison of experimental data with calculations using the semi-empirical Fuller model and the kinetic-theory Chapman–Enskog equation showed that both approaches capture the general trend of diffusion increasing with temperature, but differ significantly in accuracy and physical interpretation.

The Fuller method, based on diffusion volume correlations, demonstrates a systematic overestimation of D_{12} , especially for mixtures containing heavy and asymmetric hydrocarbons. This is due to its limited ability to account for the fine structure of molecular interactions. At the same time, the Chapman–Enskog model, which employs the Lennard–Jones potential and a microscopic description of collisions, reproduces experimental values with high accuracy (average deviation does not exceed 10–15%) and correctly reflects the influence of molecular mass, size, and nature [2, 4, 14].

The obtained results are of particular importance for engineering and computational applications. The derived temperature dependences and accuracy assessment of the models can be used in mass transfer calculations for multicomponent mixtures, modeling of combustion, gas separation and mixing processes, as well as in numerical simulations. It is shown that the combination of experimental data and the Chapman–Enskog model provides a physically grounded and quantitatively reliable description of diffusion properties, making it the preferred choice for scientific and engineering tasks.

For example, in CFD modeling of gas mixing in a natural gas pipeline or combustion chamber, the binary diffusion coefficient directly affects the predicted rate of species mixing and the thickness of concentration boundary layers. Using a diffusion coefficient overestimated by 30–40% in a CFD model can potentially lead to an artificially accelerated mixing process, which, in turn, may result in inaccurate predictions of the local fuel–air mixture composition and, consequently, the characteristics of combustion and heat transfer. This effect is particularly important for hydrocarbon-rich mixtures, for which the Fuller correlation may substantially overestimate the diffusion coefficient.

Thus, the results not only confirm the applicability of classical kinetic theories but also provide a basis for further improvement of empirical correlations that account for complex intermolecular interactions in hydrocarbon and gas systems. The presented dependencies can serve as a benchmark for future numerical studies and the development of universal models for binary diffusion in polyatomic gas mixtures.

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