The 21st International Conference on
Thermal Science and Engineering of Serbia
SimTerm 2024
Niš, Serbia, Oct 22-25 2024
doi: 10.5937/SimTerm24349P

Determining Gas and Gas Mixture Viscosity Across Wide Temperature Ranges: Refinements and Predictive Models

Jovica Podunavac[a], Nenad Tomić[b], Mladen Tomić[c], Aleksandar Anđelković[d], Miroslav Kljajić[e], Predrag Živković[f]

[a] Faculty of Technical Sciences, University of Novi Sad, RS, jovica.podunavac@gmail.com
[b] Faculty of Technical Sciences, University of Novi Sad, RS, nenadtomich@yahoo.com
[c] Faculty of Technical Sciences, University of Novi Sad, RS, mladen.tomic@uns.ac.rs
[d] Faculty of Technical Sciences, University of Novi Sad, RS, aleksa@uns.ac.rs
[e] Faculty of Technical Sciences, University of Novi Sad, RS, kljajicm@uns.ac.rs
[f] Faculty of Mechanical engineering, University of Niš, RS, predrag.zivkovic@masfak.ni.ac.rs

Abstract This study delves into refining the ideal gas viscosity equation by introducing amendments that account for temperature variations and critical temperature ratios across diverse ideal gases. The investigation involves comparing the adjusted formula with empirical data obtained from various gases under extreme conditions, including ultra-critical temperatures and near-critical points like for water and carbon dioxide. The primary objective is to enhance the equation's accuracy and applicability. The research proposes novel modifications integrating a temperature-dependent dumping coefficient and a redefined temperature exponent. These adjustments aim to capture gas behavior across a wider spectrum of temperatures, pressures, and gas compositions. Building upon foundational works in gas dynamics and molecular theory, this study bridges the gap between theoretical formulations and empirical observations. To validate these modifications, empirical data from gases under diverse conditions, including ultra-critical temperatures and mixtures, were utilized. Notably, the study's focus extends to analyzing gases under extreme conditions, highlighting the formula's improved predictive capability, and assessing its performance against complex gas mixtures using software-generated data. The findings reveal that these proposed adjustments significantly enhance the equation's alignment with real-world observations. Specifically, the analysis showcases improved predictive accuracy, especially in extreme gas conditions, and promising results when evaluating complex gas mixtures. These modifications offer a more comprehensive framework for estimating viscosity across a broad range of gas types and conditions, thereby enhancing the predictive power of the ideal gas viscosity equation.

Keywords: Gas Mixture, Real Gases, Temperature-Dependent, Viscosity.

1 Introduction

Viscosity, a fundamental property governing the resistance of fluids to flow, holds paramount importance across of scientific and industrial domains. From facilitating efficient energy conversion processes in power generation to optimizing fluid dynamics in chemical engineering applications, understanding and accurately predicting viscosity is crucial for ensuring optimal performance and reliability. However, conventional viscosity equations, particularly those applicable to ideal gases, often encounter limitations when confronted with real-world complexities, necessitating refinements to enhance their predictive capabilities and broaden their applicability across diverse operating conditions. The theoretical foundation for estimating viscosity in ideal gas states is deeply rooted in the pioneering contributions of Chapman, who laid the groundwork in their work [1]. Bird's influential advancements further propelled the understanding of gas behavior and viscosity calculations [2].

Despite the efficacy of the ideal gas viscosity equation as a foundational tool, its practical applicability encounters inherent limitations, particularly in scenarios involving real-world complexities. Gases operating under extreme conditions or within intricate mixtures present challenges beyond the predictive capacity of conventional equations. Addressing these limitations requires a nuanced approach, prompting an in-depth exploration aimed at refining the ideal gas viscosity equation.

Precise characterization of fluid flows is essential and requires accurate estimations of bulk viscosity, particularly evident in systems like Rankine cycle power systems utilizing steam and those employing non-aqueous working fluids. The latter proves advantageous in scenarios involving non-fossil fuel heat sources. Noteworthy studies, conducted by researchers focus on organic Rankine cycles, examining their efficiency and

performance [3-7]. These investigations contribute to a comprehensive understanding of fluid flow behaviors in various applications, spanning traditional power systems to eco-friendly energy sources.

This study embarks on proposing innovative modifications to the existing equation to better account for variations in temperature and critical temperature ratios across diverse ideal gases. These proposed amendments seek to introduce a temperature-dependent coefficient and redefine the temperature exponent, intending to capture the intricacies of gas behavior over a broader spectrum of temperatures, pressures, and compositions.

The objective of this research is twofold: firstly, to bridge the theoretical and empirical gap between molecular-level interactions and macroscopic observations within gases, and secondly, to enhance the equation's accuracy and applicability in diverse real-world scenarios. By reconciling theoretical formulations with empirical data, this study aims to develop more precise viscosity equations, aligning them more closely with observed behaviors and intricate molecular dynamics within gases.

To validate the efficacy of these proposed modifications, data obtained from various gases under extreme conditions, including those operating at ultra-critical temperatures and near-critical points such as water and carbon dioxide, will be meticulously analyzed. Moreover, the assessment will extend to include complex gas mixtures, utilizing software-generated data to evaluate the versatility and predictive power of the modified equation.

The ultimate aspiration of this research lies in cultivating an enhanced ideal gas viscosity equation that can robustly estimate viscosity across a wide range of gas types and conditions, thereby refining predictive models and enabling more accurate estimations of viscosity in intricate real-world scenarios.

2 Fundamentals of Viscosity in Ideal Gases

Viscosity in ideal gases, as envisioned by kinetic and molecular theory, is intricately tied to the dynamic behavior of gas molecules. This theory posits that viscosity emerges from the complex interplay of various molecular properties. Central to this understanding are factors such as the average speed of gas molecules, the density of the gas, and the mean free path—the average distance traveled by a molecule between collisions.

The average molecular speed within a gas directly influences its viscosity. Higher speeds lead to increased molecular collisions and, consequently, greater resistance to flow. Density also plays a pivotal role, affecting the frequency of molecule-to-molecule interactions. Higher densities result in more frequent collisions, impacting the overall viscosity of the gas.

Additionally, the mean free path, representing the average distance traveled by molecules between collisions, is crucial. Shorter mean free paths imply more frequent collisions, increasing resistance to flow. At the molecular level, properties like the kinetic diameter of molecules and their individual masses further influence viscosity. Larger molecules or those with greater mass might exhibit different collision behaviors, impacting the overall viscosity of the gas.

Temperature stands as a critical parameter in this framework. Its influence on viscosity is multifaceted, altering molecular speeds and collision frequencies. Typically, as temperature increases, molecular speeds rise, potentially reducing viscosity due to heightened molecular motion.

The intricate relationship between these molecular properties and their effects on the macroscopic behavior of gases forms the foundation of understanding viscosity in ideal gases. Refining viscosity equations involves reconciling these molecular-level interactions with macroscopic observations, aiming to create more accurate models that encapsulate the behavior of gases across a broad spectrum of conditions

The relationship is commonly expressed through the kinetic theory equation for viscosity, which in its simplest form for an ideal gas can be represented as:

$$\mu = \frac{1}{3} \cdot \rho \cdot \bar{w} \cdot \bar{l}, \tag{1}$$

where:

- μ is the viscosity of the gas [Pa·s],
- ρ is the density of the gas [kg·m-3],
- $\bar{w}$ is the average molecular speed [m/s],
- $\bar{l}$ is the mean free path [m].

This equation highlights the fundamental factors contributing to gas viscosity as per the kinetic theory. The viscosity (μ) is directly proportional to the density (ρ) and the mean free path ($\bar{l}$), while it is also related to the average molecular speed ($\overline{w}$) of the gas molecules, or according to the kinetic and molecular theory in different form [7]:

$$\mu = \frac{2}{3} \cdot \frac{\sqrt{m_c \cdot k \cdot T}}{\pi^{1.5} \cdot d^2}, \tag{2}$$

where:

- m_c is the mass of the molecule [kg],
- k is the Boltzmans constant,
- d is the kinetic diameter of the molecule [m],
- T is the absolute temperature [K].

which can be written taking all the constants on one side as:

$$\mu = C \cdot \sqrt{T}. \tag{3}$$

Upon examining ideal gases operating significantly distant from their critical temperatures, notable disparities emerge between empirical measurements and theoretical predictions, as presented in the Fig 1. on the example of hydrogen.

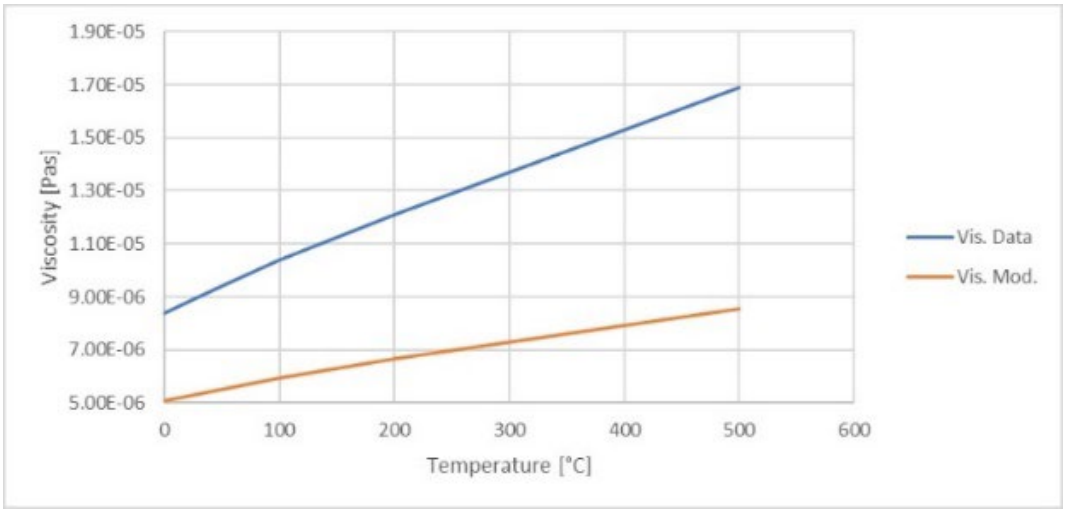

Figure 1 Comparison between modeled values and actual data for hydrogen

3 Temperature-Dependent Deviations and Model Refinements

The discrepancy between the ideal gas viscosity predicted by the kinetic theory and real-world data often necessitates adjustments to the temperature exponent in the viscosity equation [8,9]. Empirical observations reveal that a modification, typically involving a temperature exponent ranging between 0.50 to 0.7, is required to align theoretical predictions more closely with experimental results.

This adjustment acknowledges that the standard kinetic theory-based viscosity equation, which assumes a temperature exponent of 0.5, might not sufficiently encapsulate the intricate temperature dependence observed in real gas behavior. The need for a higher temperature exponent suggests that molecular interactions and collision dynamics within gases, especially under varying temperatures, might deviate from the simplistic assumptions inherent in the classical kinetic theory formulations. Thus, modifying the temperature exponent serves as a means to bridge the gap between theoretical predictions and observed real-world data, refining the equation to better represent the complexities of gas behavior across a broader temperature range. The empirical evidence strongly advocates for an adjustment in the temperature exponent to 0.583 to better harmonize theoretical predictions with experimental data under these conditions, as illustrated with Fig. 2 and recalculated viscosity of hydrogen.

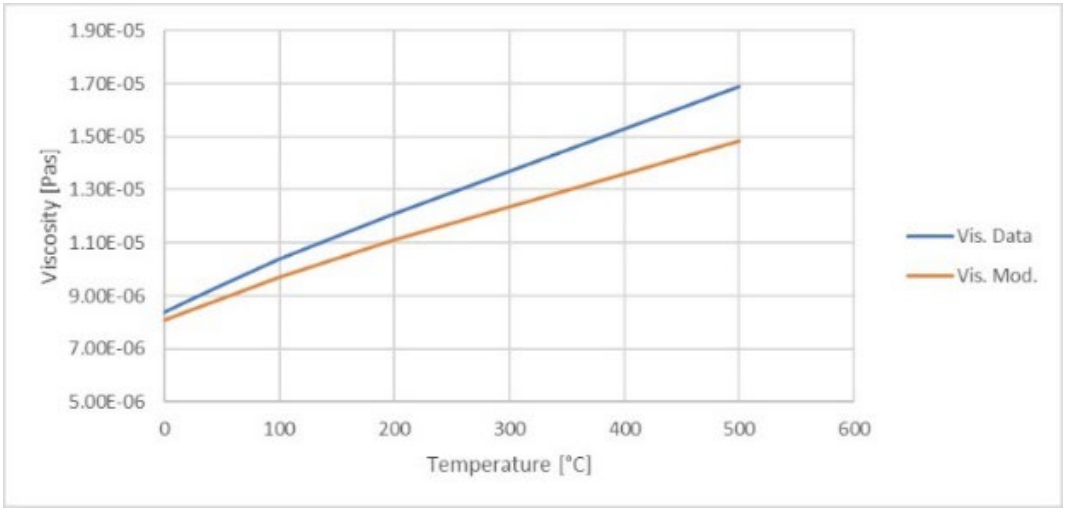

Figure 2 Comparison between modeled values with adjasted exponent and actual data for hydrogen

The comprehensive analysis conducted across a diverse array of ideal gases and mixtures has showed trends in viscosity behavior. Comparative assessments involving literature data and results generated through professional software across gases including methane, hydrogen, nitrogen, oxygen, flue gases, methane-air mixtures, and carbon dioxide have unveiled pivotal insights into viscosity variations relative to temperature ratios concerning critical temperatures.

The analysis highlights a critical divergence from conventional kinetic theory assumptions, particularly for temperature ratios lower than 5 as illustrated in Fig. 3.

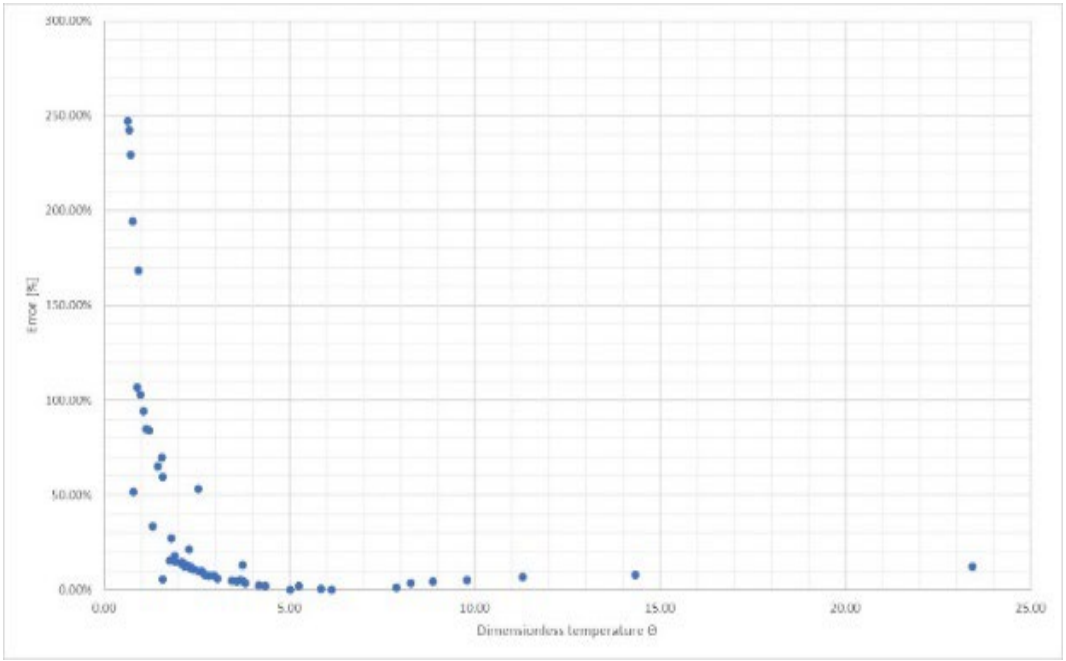

Figure 3 Deviation as a function of dimensionless temperature

Moreover, the observed equivalence between mass and kinetic diameter, when compared against mol-averaged values within these mixtures, implies a coherent behavior in viscosity calculations. This alignment between mixed gases and averaged properties suggests a potential avenue for simplification in modeling gas mixtures, showcasing the viability of using averaged values to achieve accurate viscosity predictions:

$$\mu = \frac{2}{3} \cdot \frac{\sqrt{m_{cm} \cdot k}}{\pi^{1.5} \cdot d_m^2} \cdot T^{0.583}, \tag{4}$$

where for the mixtures of *n* components:

$$m_{cm} = \sum_{i=1}^{n} r_i \cdot m_{ci},$$
$$d_m = \sum_{i=1}^{n} r_i \cdot d_i, \quad (5)$$

where r_i represents the molar/volume share of the i-th component in ideal gas. The results for some ideal gases mixtures gases are presented in Fig. 4 and 5.

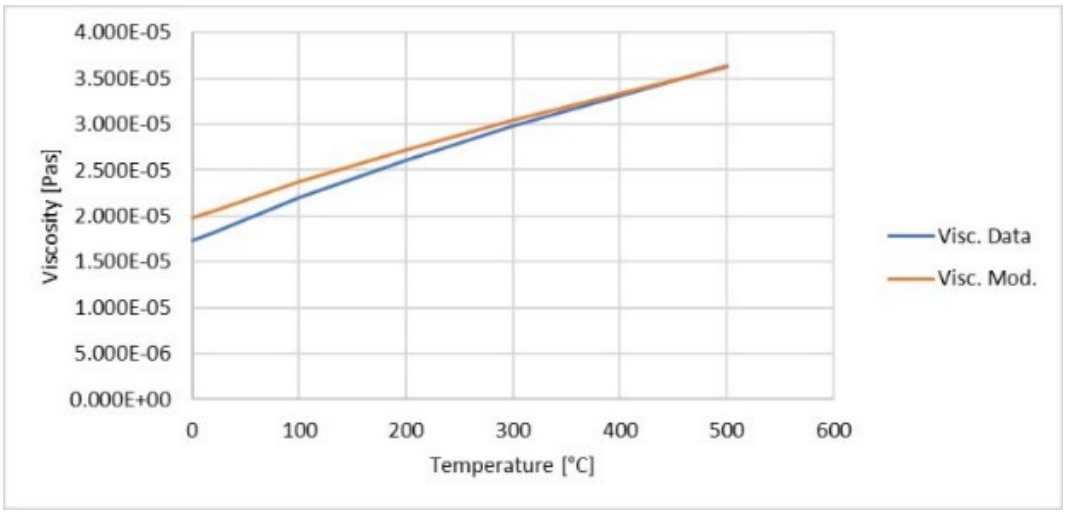

Figure 4 Comparison between modeled values with adjusted exponent and actual data for mixture – air

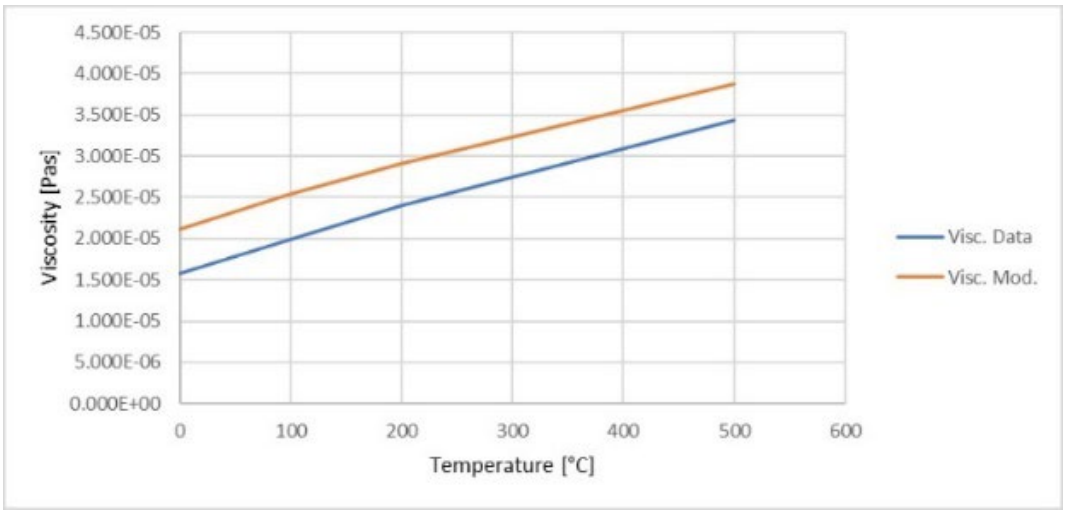

Figure 5 Comparison between modeled values with adjusted exponent and actual data for mixture – flue gases

The comparisons for ultracritical gasses show good agreement, while for gases close to critical point for ratio under 4 are significant differences with error less than 11% and average error under 7%., while for the gasses as carbon dioxide the difference was significant. Also, for critical temperature ratio over 20 the error starts rising again.

Expanding the applicability of the gas viscosity determination equation to near-critical regions, as well as to make an additional correction, a corrective coefficient has been introduced, accounting for the proximity to the critical temperature as a factor influencing viscosity. The correction factor is equal to:

$$\beta = -1.1018 \cdot 10 - 41.01655 \cdot \frac{\Theta^{1.83565}}{1.0223128 + \Theta^{1.83565}}, \quad (6)$$

where $\Theta = \frac{T}{T_c}$, where the Tc represents a critical temperature, thus

$$\mu = \beta \cdot \frac{2}{3} \cdot \frac{\sqrt{m_{ce} \cdot k}}{\pi^{1.5} \cdot d_e^2} \cdot T^{0.583}. \quad (7)$$

The critical temperature of a mixture refers to the highest temperature at which the liquid and gas phases of the mixture can coexist in equilibrium. It's a characteristic property of the mixture and is influenced by the individual critical temperatures of its components as well as their proportions. To estimate the critical temperature of this mixture, one can use a simple mixing rule like the arithmetic average:

$$T_{cm} = \sum_{i=1}^{n} r_i \cdot T_{ci}. \quad (8)$$

The results show good agreement between predicted viscosity of gases and gas mixtures for temperatures ratio of 2.0., but for most gases which are considered ideal even closer to ratio of 1.5. The general correlation between model and literature values is presented in the Fig.6.

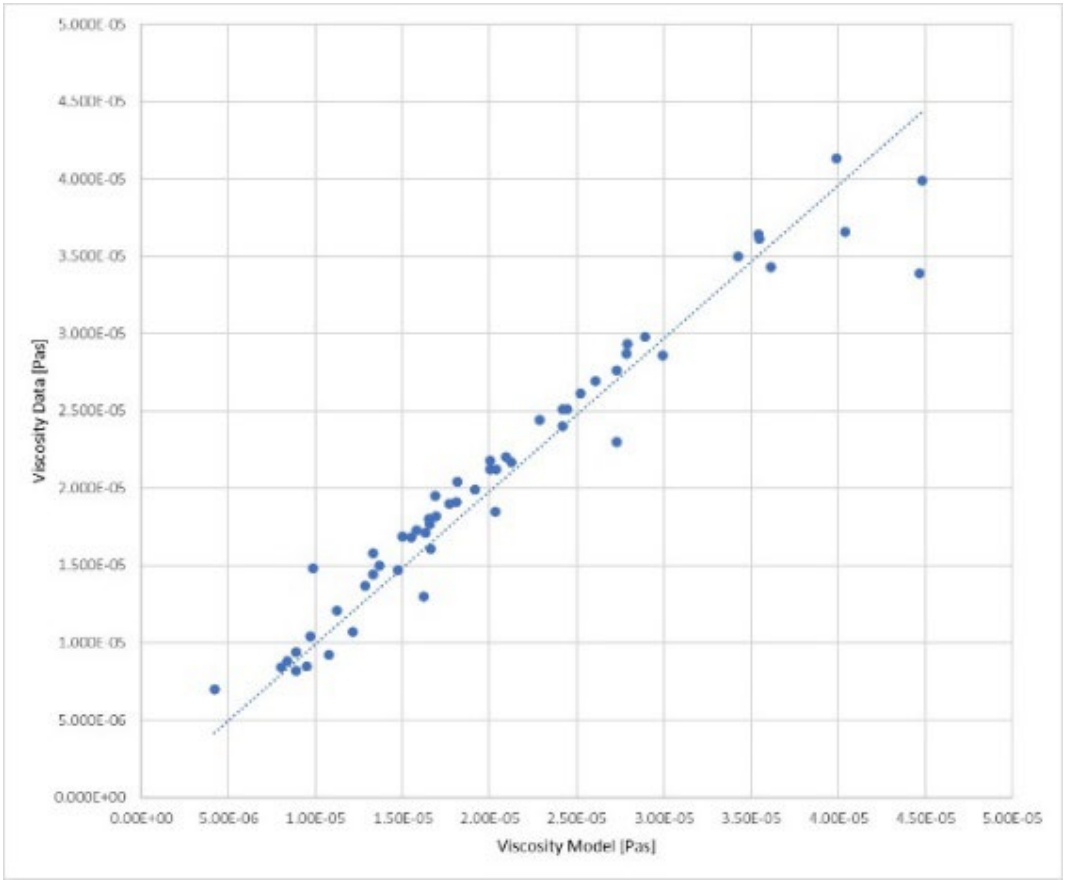

Figure 6 Correlation between modeled values and actual data

4 Conclusion

A simple method has been developed for calculating the viscosity of a mixture of gases. The development relies on additive contributions of molecule masses and its volume fraction momentum fraction as the primary compositional variable. A single global empirical constant is used in this model, which can be easily applied to near critical regions of fluids. The only data required by this equation to calculate viscosity for a known composition mixture are the molecular weights and critical temperatures of the pure components at the given temperature and pressure. For most binary gas mixtures, this equation performs at least as well as the best available method using comparable data.

Collectively, these findings underscore the imperative for refined adjustments in viscosity equations to accommodate diverse temperature dependencies, particularly in gases operating at elevated temperature ratios. Additionally, the implications of equivalences observed in mixed gases and averaged properties highlight the potential for streamlined modeling approaches in complex gas mixtures. This research significantly contributes

to advancing our understanding of viscosity estimations across a wide spectrum of gases and mixtures under diverse conditions, paving the way for enhanced predictive models in fluid dynamics and engineering applications.

References

[1] S. Chapma, T. G. Cowling, Mathematical Theory of Non-uniform Gases, *Cambridge university press,* Cambridge, UK, 1991
[2] G. A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, *Clarendon,* Oxford, UK, 1994
[3] M. S. Cramer, Numerical estimates for the bulk viscosity of ideal gases, Physics of Fluid, *24* (2012), pp. 066102
[4] B. T. Liu, K. H. Chien, and C. C. Wang, Impact of working fluids on the organic Rankine cycle for waste heat recovery, Energy, *29* (2004), pp. 1207-1217
[5] D. Wei, X. Lu, Z. Lu, and J. Gu, Analysis and optimization of the performance of the organic Rankine cycle (ORC) for waste heat recovery, Energy Convers. Manage., *48* (2007), pp. 1113-1119
[6] B. Saleh, G. Koglbauer, M. Wendland, and J. Fischer, Working fluids suitable for low-temperature organic Rankine cycles, Energy, *32* (2007), pp. 1210-1221
[7] A. Shuster, S. Karellas, and R. Aumann, Potential efficiency optimization in supercritical organic Rankine cycles, Energy, *35* (2010), pp. 1033
[8] N. Radojković, G. Ilić, M. Vukić, I. Stojanović, P. Živković, Termodinamika II, 2nd ed., *Mašinski fakultet Niš, Niš*, Niš, Serbia, 2007.
[9] ***, https://www.engineeringtoolbox.com/ (as acessed on 01.11.2024)
[10] M. Tomić, M. Vukić, P. Živković, B. Milutinović, Zbirka zadataka iz termodinamike sa osnovama prenosa toplote, *Fakultet tehničkih nauka Novi Sad,* Novi Sad, Serbia, 2021