Understanding Isomeric Effects on Properties of Aviation Fuels via a Group Contribution Method

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National Laboratory of the Rockies

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Understanding isomeric effects on properties of aviation fuels via a group contribution method

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Abstract: The molecular composition of aviation fuels, including conventional and sustainable aviation fuels (SAFs), significantly influences their performance, safety, and environmental impact. This study examines the effect of isomeric variation for compounds with the same carbon number and chemical family on key fuel properties, focusing on compounds commonly found in conventional jet fuels and SAFs. A group contribution method (GCM) is employed to predict thermophysical and combustion properties, providing an efficient analytical approach to evaluate the contributions of individual compounds to overall fuel mixture behavior. As part of this work, we introduce FuelLib, an open-source Python tool built around the GCM, to calculate individual compound and fuel mixture properties using various mixing rules. Our work evaluates whether the GCM can capture isomeric effects, which are often overlooked in traditional fuel property estimation. This is particularly important for SAFs, which are often made up of fewer compound classes than conventional fuels, making the impact of isomeric differences more pronounced. Two-dimensional gas chromatography (GCxGC) data, which can be obtained from small fuel samples, provides weight percentages of compounds grouped by chemical family and carbon number rather than detailed information about individual compounds. As a result, assumptions must be made when decomposing GCxGC data into individual compounds with defined functional groups for GCM applications. Using GCxGC data, we show that the FuelLib tool can be used to predict the fuel properties of conventional jet fuels, with validation against experimental data. The provided tool enables researchers to predict fuel properties of candidate fuels and supports the design of new SAFs at both the component and mixture levels. This capability provides a foundation for studying fuel and combustion properties during SAF development, reducing reliance on costly experimental methods and advancing progress toward certification of new SAFs.

Keywords: Fuel property prediction, Sustainable aviation fuel, Group contribution method, Isomeric effects

1. Introduction

The Group Contribution Method (GCM), specifically the method introduced by Constantinou and Gani in the mid-1990s [1, 2], offers a systematic approach for estimating the thermodynamic properties of pure organic compounds. This method decomposes molecules into structural groups, each associated with predefined contributions to specific properties. By summing these contributions, GCM enables the prediction of key thermodynamic properties under standard temperature and pressure conditions. This predictive capability is particularly advantageous for complex mixtures, especially when experimental thermodynamic data is unavailable. One example is sustainable

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aviation fuels (SAFs), which frequently lack comprehensive thermodynamic datasets. The GCM serves as a valuable tool for estimating these properties, facilitating the evaluation of potential fuel compositions without the need for extensive experimental testing, thus expediting the development of viable SAFs.

Despite its well-established use in chemical engineering (e.g., the UNIFAC model [3] for phase equilibria) and spread to adjacent fields such as biophysics [4], the application of GCM in SAF end use research remains relatively limited. One notable contribution is the work by Govindaraju and Ihme [5], who developed a GCM-based framework for predicting multicomponent evaporation rates in jet fuels. Their approach made use of the inherent functional groups and relative weight percentages of the fuel components, as derived from two-dimensional gas chromatography (GCxGC) data, where the weight composition is categorized into hydrocarbon families. However, their framework relied on assumptions about reference compounds representing each hydrocarbon family in the GCxGC data. This simplification raises questions about the extent to which isomeric effects—variations within these hydrocarbon families—are captured and how such effects could propagate into mixture property estimates.

More recently, Hall et al. [6] analyzed a dataset of 1,870 jet-range hydrocarbons, investigating nine important fuel properties with a focus on the effects of isomerization, carbon number, and molecular structure. Their findings revealed that isomeric variance has a more significant influence on freeze point and viscosity than hydrocarbon family or carbon number, emphasizing the importance of accounting for isomeric effects in fuel property modeling. They proposed that the success of fuel property predictions based on GCxGC data for conventional jet fuels stems from the extensive isomeric diversity among the thousands of compounds within the fuel, which drives the properties of hydrocarbon groups with many isomers to converge toward the mean. However, for SAFs, where isomeric diversity is more limited, they caution that the predictive reliability of such methods diminishes significantly. These results have practical implications for ASTM D4054 [7] fuel approval processes and future fuel design, particularly for SAFs.

Using computational fluid dynamics, Nadakkal Appukuttan et al. [8] demonstrated that liquid properties of SAFs can have a significant effect on the fuel vaporization process and eventual distribution of fuel in a realistic aviation gas turbine combustor. Therefore, to assess the potential viability of new SAF pathways through combustor simulations, it is essential to have accurate property prediction capability, despite the fuels being complex mixtures for which measurements at the relevant conditions may not be practical. This work builds toward a capability based on GCxGC measurements coupled to the GCM that would enable accurate property estimation for new SAF pathways. Specifically, it examines key fuel properties for compounds commonly found in both conventional jet fuels and SAFs. Our study evaluates whether GCM can effectively capture isomeric effects and propagate them into mixture property estimates. The eventual objective is to implement this approach in the spray module of the PelePhysics library [9] to allow for combustor simulations in the PeleLMeX flow solver [10, 11] that was used by Nadakkal Appukuttan et al. [8]

2. Methods

2.1 The Group Contribution Method

The GCM is implemented using *FuelLib* [12], which builds on Govindaraju's [13] Matlab implementation of the GCM, and incorporates gas chromatography data from the Air Force Research

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Laboratory (AFRL) [14]. It extends the original functionality by calculating additional thermodynamic and mixture properties using GCM property predictions from individual compounds. The GCM prediction process works as follows. For a mixture of N_c compounds, let $\mathbf{N}$ be an $N_c \times N_{g_1}$ matrix that represents the number of first-order groups in each compound, where N_{g_1} is the total number of first-order groups as defined by Constantinou and Gani [1, 2]. Similarly, let $\mathbf{M}$ be an $N_c \times N_{g_2}$ matrix that specifies the number of second-order groups in each compound, where N_{g_2} is the total number of second-order groups. The GCM property predictions for the i^{th} compound in the mixture, under standard temperature and pressure conditions, are calculated following the method described by Constantinou and Gani [1, 2]:

$$M_{w,i} = \left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} m_{w1k}\right] \times 10^{-3} \quad [\text{kg/mol}], \tag{1}$$

$$T_{b,i} = 204.359 \ln\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} t_{b1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} t_{b2j}\right] \quad [\text{K}], \tag{2}$$

$$T_{c,i} = 181.28 \ln\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} t_{c1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} t_{c2j}\right] \quad [\text{K}], \tag{3}$$

$$\mathrm{p}_{c,i} = \left(\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} \mathrm{p}_{c1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} \mathrm{p}_{c2j} + 0.10022\right]^{-2} + 1.3705\right) \times 10^5 \quad [\text{Pa}], \tag{4}$$

$$\Delta H_{v,\mathrm{stp},i} = \left(\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} h_{v1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} h_{v2j}\right] + 6.829\right) \times 10^3 \quad [\text{J/mol}], \tag{5}$$

$$V_{m,\mathrm{stp},i} = \left(\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} v_{m1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} v_{m2j}\right] + 0.01211\right) \times 10^{-3} \quad [\text{m}^3/\text{mol}], \tag{6}$$

$$\omega_i = 0.4085 \ln\left(\left[\sum_{k=1}^{N_{g_1}} \mathbf{N}_{ik} \omega_{1k} + \sum_{j=1}^{N_{g_2}} \mathbf{M}_{ij} \omega_{2j} + 1.1507\right]^{1/0.5050}\right). \tag{7}$$

Here, $M_{w,i}$ is molecular weight, $T_{b,i}$ is normal boiling point, $T_{c,i}$ is critical temperature, $\mathrm{p}_{c,i}$ is critical pressure, $\Delta H_{v,\mathrm{stp},i}$ is enthalpy of vaporization, $V_{m,\mathrm{stp},i}$ is liquid molar volume, and ω_i is the acentric factor. The lowercase variables in the corresponding summations denote the specific first- and second-order group contributions as tabulated by Constantinou and Gani [1, 2].

From these estimates, relationships are used to calculate the density, viscosity and vapor pressure for the i^{th} component of the mixture, which are then combined to determine mixture properties. The mixture density is given by:

$$\rho = \sum_{i=1}^{N_c} Y_i \frac{M_{w,i}}{V_{m,i}} \quad [\text{kg/m}^3], \tag{8}$$

where Y_i is the mass fraction for compound i and the molar volume, $V_{m,i}$, is calculated at a specific temperature T using the generalized Rackett equation [15, 16] with an updated ϕ_i parameter [5]:

$$V_{m,i} = V_{m,\mathrm{stp},i} Z_{c,i}^{\phi_i}, \tag{9}$$

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where

$$Z_{c,i} = 0.29056 - 0.08775\omega_i, \tag{10}$$

$$\phi_i = \begin{cases} (1-T_{r,i})^{2/7} - (1-T_{r,\mathrm{stp},i})^{2/7}, & \text{if } T \le T_{c,i} \\ -(1-T_{r,\mathrm{stp},i})^{2/7}, & \text{if } T > T_{c,i} \end{cases}, \tag{11}$$

with reduced temperatures $T_{r,i} = T/T_{c,i}$ and $T_{r,\mathrm{stp},i} = T_{\mathrm{stp}}/T_{c,i}$, and standard temperature $T_{\mathrm{stp}} = 298.15$ K.

The kinematic viscosity of the i^{th} compound of the fuel, ν_i, is calculated using Dutt's equation [17] provided T and $T_{b,i}$ in °C:

$$\nu_i = 10^{-6} \times \exp\left\{ -3.0171 + \frac{442.78 + 1.6452\,T_{b,i}}{T + 239 - 0.19\,T_{b,i}} \right\} \quad [\mathrm{m^2/s}]. \tag{12}$$

The mixture kinematic viscosity is computed using the Arrhenius mixing rule [18]:

$$\ln \nu = \sum_{i=1}^{N_c} X_i \ln \nu_i, \tag{13}$$

where X_i is the mole fraction of compound i.

The saturated vapor pressure for each compound is calculated as a function of temperature using the Lee–Kesler method [19], which solves

$$\ln \mathrm{p}_{r,sat,i} = f_i^{(0)} + \omega_i f_i^{(1)}, \tag{14}$$

to obtain the reduced saturated vapor pressure $\mathrm{p}_{r,sat,i} = \mathrm{p}_{sat,i}/\mathrm{p}_{c,i}$. The critical pressure and acentric factor are calculated by Equations (4) and (7), respectively. The temperature-dependent terms $f_i^{(0)}$ and $f_i^{(1)}$ are defined as:

$$f_i^{(0)} = 5.92714 - \frac{6.09648}{T_{r,i}} - 1.28862 \ln T_{r,i} + 0.169347\,T_{r,i}^6, \tag{15}$$

$$f_i^{(1)} = 15.2518 - \frac{15.6875}{T_{r,i}} - 13.4721 \ln T_{r,i} + 0.43577\,T_{r,i}^6. \tag{16}$$

Finally, the mixture vapor pressure is calculated according to Raoult's law:

$$\mathrm{p}_v = \sum_{i=1}^{N_c} X_i\, \mathrm{p}_{sat,i} \quad [\mathrm{Pa}]. \tag{17}$$

2.2 Evaluating Isomeric Effects

This study evaluates the ability of the GCM to capture isomeric effects within hydrocarbon family groups, focusing on a subset of compounds analyzed by Hall et al. [6]. The 55 compounds examined in this study are categorized by family and carbon number in Table 1. Except for the mono-cyclo-alkanes, where 1,3-di-tert-butylcyclohexane was excluded due to insufficient reference data, the compounds align with those in the supplementary material of Hall et al. [6].

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Family	Carbon number	Number of isomers
iso-alkanes	8	18
mono-cyclo-alkanes	14	16
bi-cyclo-alkanes	14	16
tri-cyclo-alkanes	14	5

Table 1: The four hydrocarbon families and carbon numbers of the 55 compounds studied.

For each compound, GCM property predictions were computed and compared qualitatively to predictive values from the NIST Standard Reference Database 203 Web Thermo Tables [20]. Figure 1 shows an example of the agreement between GCM and NIST predictions for the boiling points of the 16 mono-cyclo-alkanes, normalized by the median GCM prediction of boiling point across all mono-cyclo-alkane compounds. Throughout, the discrepancies between the predictions were typically small relative to the property variation between different isomers in the same class, indicating satisfactory performance of the GCM for capturing isomeric variation. To evaluate this in more detail across a wider range of compounds and properties, the extrema and averages of the GCM and NIST predictions were calculated across individual hydrocarbon families to evaluate whether the GCM effectively captured the isomeric ranges observed in the NIST predictions and in the measurement data reported by Hall et al.[6].

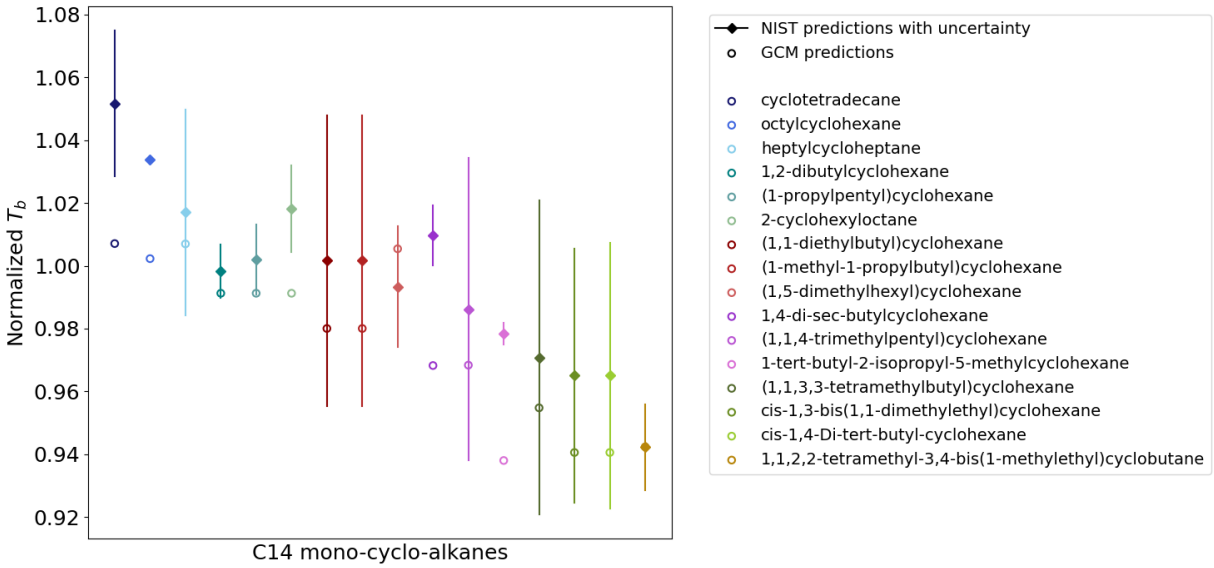

Figure 1: Normalized GCM predictions of boiling point for the 16 C14 mono-cyclo-alkanes against predictions from NIST [20].

In addition to evaluating property predictions for single compounds and individual compound classes, we also do preliminary evaluations of the GCM predictions for real fuels that are complex mixtures of many types of compounds. Mixture density, viscosity and vapor pressure were calculated for three conventional jet fuels (JP-5, JP-8, and Jet A) over a range of temperatures. The fuels were represented using GCxGC data from AFRL [14], which provides weight percentages of hydrocarbon families by carbon number. Reference compounds were decomposed into func-

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tional groups to represent the hydrocarbon families. The selection of reference compounds was somewhat arbitrary in order to evaluate the GCM predictions based on GCxGC data when further data about which isomers are actually present for each carbon number and family. Typically, the simplest possible compound within each group would be selected as a reference. For example, monocycloalkanes would be decomposed as a six-membered ring with a single straight alkane side chain (i.e., n-butylcyclohexane for a C10 monocycloalkane, etc.). The calculated mixture properties were then compared to measurement data from the AFRL [14].

3. Results and Discussion

Averages and variance in property values for the 55 compounds are presented for GCM predictions, NIST predictions [20], and the measurement data from Hall et al. [6] in Figures 2, 3 and 4. While the GCM predictions qualitatively capture the overall trends and the isomeric variance within each hydrocarbon family, the averages generally underpredict the data. As expected, most hydrocarbon families show limited variance in vapor pressure and freezing point (not shown). The poorest agreement is observed for tri-cyclo-alkane compounds, which are relatively rare in actual jet fuels.

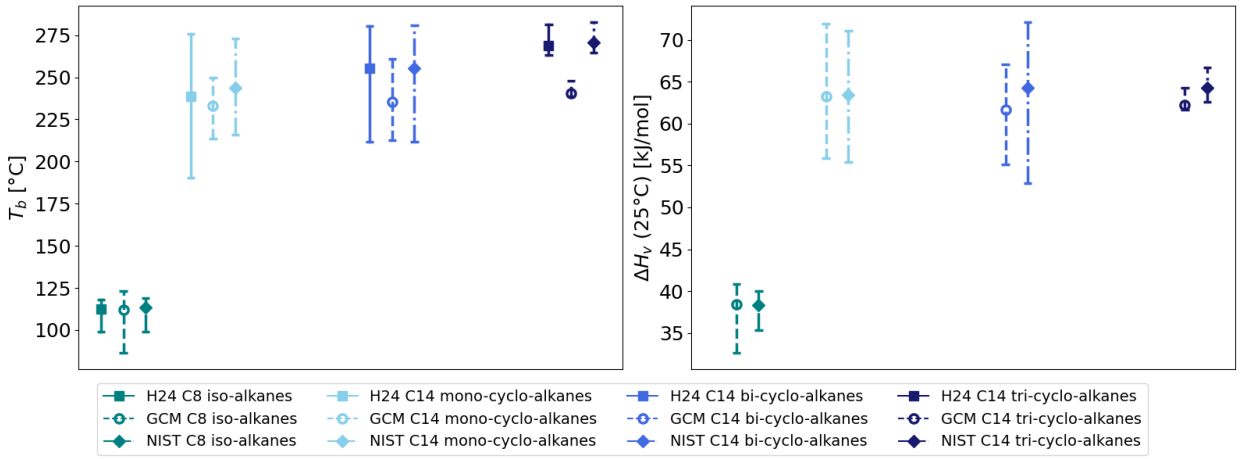

Figure 2: Normal boiling point (left) and enthalpy of vaporization at 25°C (right) for select hydrocarbon families and carbon number against measurement data from Hall et al. [6] and predictions from NIST [20].

The difference in predictive accuracy between properties is largely attributable to how they are calculated. Boiling point, enthalpy of vaporization, critical temperature, and critical pressure are all computed directly from pre-tabulated group contribution values. In contrast, kinematic viscosity is calculated using Dutt's equation (12), a relationship that relies on boiling point. While the GCM generally performs well in capturing the isomeric effects on boiling point, the average boiling point for each family tends to be lower than the NIST [20] and Hall et al. [6] data, and as a result, the viscosity predictions exhibit systematically lower averages compared to the data. This dependence highlights the sensitivity of viscosity predictions to the boiling point and the need for further refinement of viscosity estimation methods.

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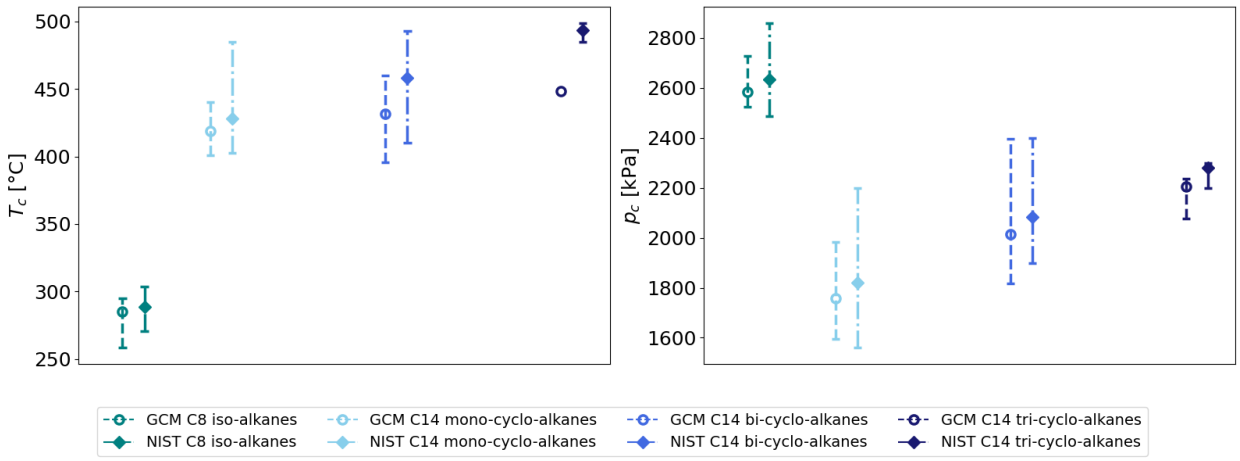

Figure 3: Critical temperature (left) and critical pressure (right) for select hydrocarbon families and carbon number against predictions from NIST [20].

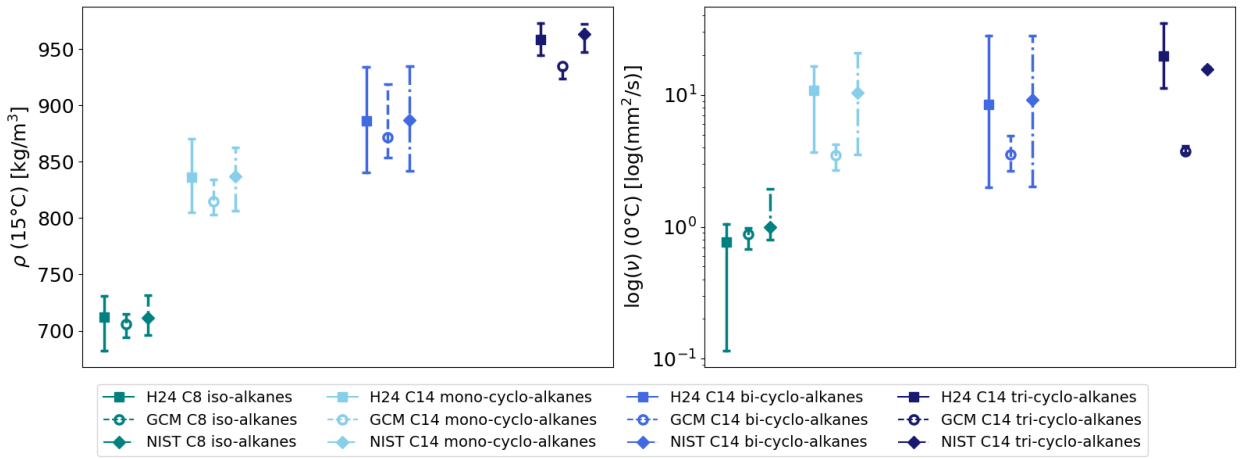

Figure 4: Density (left) and viscosity at 25 °C (right) for select hydrocarbon families and carbon number against measurement data from Hall et al.[6] and predictions from NIST[20].

The primary objective of this research is to evaluate the utility of the GCM for predicting the properties of multicomponent fuels using only GCxGC data. GCM predictions of mixture density, viscosity, and vapor pressure as functions of temperature are compared to experimental measurements from AFRL [14] in Figure 5. Despite the consistent underprediction of density for individual compounds, the GCM provides excellent agreement with experimental measurements for mixture density. Mixture viscosity predictions also demonstrate a high level of accuracy across the studied temperature range, with the exception of very low temperatures. These low-temperature discrepancies are particularly relevant for SAF qualification, as low-temperature viscosity is one of the most commonly failed specifications, but remains less well studied.

Vapor pressure predictions are equally important due to the relationship with fuel volatility. The GCM performs well in predicting mixture vapor pressure at lower temperatures but deviates from experimental data at higher temperatures. This is critical because excessive volatility at elevated temperatures can lead to operational issues such as vapor lock. These results demonstrate

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that even in the absence of detailed compositional information for specific compounds within each carbon number and hydrocarbon class, the GCM provides accurate predictions of mixture density across a wide temperature range, viscosity at higher temperatures, and vapor pressure at lower temperatures. However, a key question remains: given the relatively low number of compounds and isomers in SAFs compared to conventional jet fuels, can the GCM reliably predict SAF properties? Addressing this will require further research into the unique compositions of SAFs and their impact on fuel property predictions within the GCM framework.

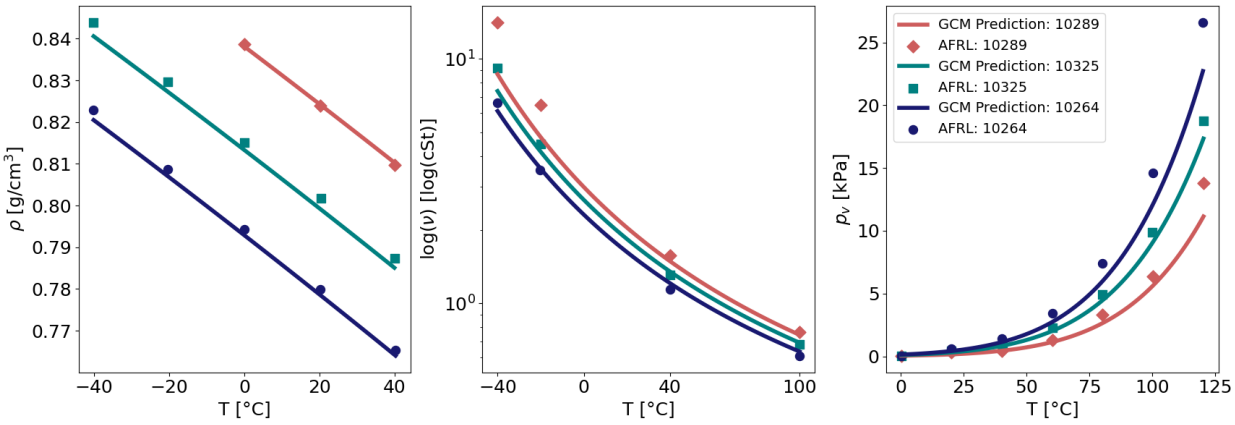

Figure 5: Density (left), viscosity (middle) and vapor pressure (right) for jet fuels POSF10289, POSF10325, and POSF10264 against data from AFRL [14].

4. Conclusions

This study introduced *FuelLib*, an open-source tool designed for predicting the thermodynamic properties of pure organic compounds and multicomponent mixtures. By leveraging the Group Contribution Method (GCM), the tool enables property estimation for complex fuels using GCxGC data and decompositions of organic compounds into fundamental groups. Though this research focused on a subset of compounds representative of those found in aviation fuels, the findings demonstrate that the GCM can capture isomeric effects, with the most accurate predictions observed for critical pressure and enthalpy of vaporization. Additionally, the study highlights the potential of GCM for estimating conventional multicomponent jet fuel properties, even in the absence of detailed molecular-level composition information. Improving predictive accuracy may be obtained by updating tabulated coefficients to better reflect aviation fuel compounds and refining the selection of reference compounds for fuels characterized by GCxGC data. Additionally, further research is needed to evaluate the reliability of GCM predictions for SAFs, given their more limited compositional diversity.

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