

Freezing Point of Hydrocarbon Fuels from Single Species Concentrations

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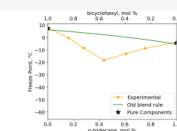


Supporting Information

ABSTRACT: The freezing point is an important property for determining the operating range of liquid hydrocarbon fuels. Many thermodynamic properties, like density, viscosity, and vapor pressure, have simple blending rules that can accurately predict the properties of a complex mixture. Freezing point, however, does not behave this way and shows nonlinear and noncontinuous responses to mixture composition. As a result, available models for freezing point predictions are generally not very effective on fuel compositions that are dissimilar to petroleum fuels. In this work, we explore a thermodynamically derived equation of state model predicting the freezing point to develop a method to predict the freezing point of mixtures from composition. The freezing point is primarily determined by the first species to freeze. Experimental control curves are used to replace complex equations to simplify the thermodynamic model. These control curves function as a strong first-order prediction of the freezing point (mean absolute error = 4.4 °C). The remaining uncertainty is attributed to the solvency effect caused by the entropy of the mixing term in the thermodynamic derivation. Utilizing the findings from this research, a 100% *n*-alkane fuel with a freezing point of −40.7 °C is blended. Using previous models built around data from conventional fuels, the closest prediction out of nine models was −12.8 °C, a 27.9 °C error. The proposed approach predicts −44.1 °C.

Empirical Models

Fail when composition of solid phase varies with blend fraction

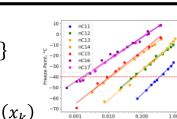


Proposed Model

$$T_{Freeze, Mixture} = \max\{T_{Freeze, k}\}$$

$$T_{Freeze, k} = f(\text{mole fraction of } k)$$

$$T_{Freeze, k}(x_k)$$



1. INTRODUCTION

The freezing point of a petroleum-refined fuel has traditionally been regarded as a difficult property to predict with confidence. These challenges are amplified when applied to synthetic fuels. One of the numerous factors contributing to this is that the freezing point is very sensitive to the hydrocarbon structure.¹ For example, 2-methylheptane has a freezing point below the measurement limit of the PAC 70Xi freezing point machine used in this experiment (<−88 °C), while a different C₈H₁₈ isomer, 2,2,3,3-tetramethylbutane, is a solid at room temperature. This difference between their freeze points that can be attributed only to structure makes methods relating hydrocarbon group type compositions to the bulk mixture freezing point unreliable. Compositional relationships from the literature have used *n*-alkane concentration, aromatic concentration, and distillation curve information among other properties to try to predict the freezing point, but these methods designed around petroleum-refined fuels have been ineffective when applied to alternative fuels.^{2,3} Such fuels generally have similar ratios of isomers within groups, even though the group concentrations vary. Petroleum-refined fuels generally have “smooth” carbon number distributions peaking at C₁₁ or C₁₂. They are primarily mixtures of *n*-alkanes, isoalkanes, cycloalkanes, and alkylbenzenes, made up of over 1000 different species. The specific species with the highest concentrations are almost always *n*-alkanes. *n*-Alkanes, especially high carbon number *n*-alkanes, have been identified

qualitatively as the cause for high freezing point fuels, but this has not been translated into specific predictions.^{4–6}

For alternative fuels, the fuel composition can be dramatically different. For instance, many fuels are composed of a single hydrocarbon family. Hydroprocessed esters and fatty acids (HEFA) are primarily alkanes; cycloparaffinic kerosene (CPK-0), which is currently in the ASTM D 4054 process, is composed of cycloalkanes; synthetic aromatic kerosene (SAK) is only aromatics. Alternative fuels do not always have many species. Farnesane, the product of ASTM D 7566 Annex A3, is composed of only one species, 2,6,10-trimethyldodecane. Iso-butanol-to-jet procedures effectively produce only two species in major quantities: 2,2,4,6,6-pentamethylheptane and 2,2,4,4,6,8,8-heptamethylnonane. These types of products necessitate a freezing point prediction model that can handle major differences in composition. In this work, we seek to develop a practical model based on the fundamental physics of freezing and mixing.

In 2022, Boehm et al. published a paper proposing a thermodynamically derived method of predicting the freezing

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point of a mixture.⁷ One of the primary conclusions of this work is that the freezing point is determined by the concentration of a single controlling species, and the balance of the sample negligibly affects the freezing point. This results in another challenge observed in predicting the freezing point: that the blending rule is not linear because the relationship between freeze point and concentration is not linear and because the controlling species may differ from one fuel to another. The published empirical blending rules for the freeze point prediction of blends of petroleum-refined fuels are not effective for blends of dissimilar solutions. This will be demonstrated in more detail in this paper. Alternatively, the experimental scope of Boehm et al. was limited to mixtures having a concentration of the freezing component greater than 10% by mole. Such concentrations are higher than those of any individual hydrocarbon in conventional jet fuel. Moreover and in spite of being significantly simpler than a prior thermodynamically derived model,⁸ that model requires several thermodynamic property inputs such as enthalpy and entropy of fusion as well as liquid and solid phase heat capacities, which are not always readily available. Such an absence of inputs makes it difficult to implement in fuel-property prediction models. Adding to this inconvenience, the Boehm model is an implicit function $T = f(T, x)$ for which an iterative solution methodology is not always well-behaved.

Although the thermodynamic models^{7,8} are impractical for complex fuel predictions, the fundamentals behind them are tractable for a simpler model. Boehm's model suggests that the freezing point of a fuel is limited by the freezing point of only one molecule, which implies we only need to identify and characterize that one species to get a freezing point prediction. For a given complex fuel sample, we only need to characterize the concentrations of species with high freezing points, and we can apply the model to each of these species and logically select the maximum value from this set of interim predictions. Taking this a step further, we do not need to use a thermodynamic model to predict values. Because the balance of the hydrocarbons in the mixture was deemed unimportant, the freeze point of species k , as a function of concentration of this species, can be measured experimentally in blends with control hydrocarbons, and the resulting control curves can be used in place of the moderately complex thermodynamic model to explicitly relate freeze point of species k to its concentration in the mixture. GC \times GC/FID-VUV is perfectly suited for determining concentration of individual species in complex mixtures.⁹ All specific isomers with relatively large concentrations that have been seen before are included in the spectral database and will continue to grow as more species relevant to the freezing point are identified.

In this work, we explore the above hypothesis expanding upon the work of Boehm et al.⁷ to improve the scientific understanding of the impact of composition on freezing point. We will detail the problems associated with other freezing point models, evaluate the experimental control curve as a prediction method, and determine the accuracy of the conclusions made in Boehm et al. First, we present additional results reinforcing the theory of Boehm et al. by showing that the freezing point of blends of two high freezing point species (*n*-tridecane and bicyclohexyl) results in a decrease in freezing point, a trait that will not be predicted in most other models. Next, we test C11–C17 *n*-alkanes in iso-octane to generate reference data predicting when each of these species will freeze in a mixture at various concentrations. We use these data to

test the hypothesis when applied to synthetic fuels. Then, we perform tests to isolate the second-order effects of species interaction and blending. Finally, we leverage the results of this research to generate a 100% *n*-alkane fuel that passes the ASTM D 1655 limit for the freezing point.

2. EXPERIMENTAL SECTION

Freezing point measurements of many hydrocarbon blends are discussed. Freezing point is measured using a Phase Technology PAC 70Xi: Cloud, Pour, and Freeze Point Analyzer, following the procedure described in ASTM D 5972. The machine has a reporting resolution of 0.1 °C and can measure between –88 and 70 °C. 0.15 mL samples are injected into a metallic sample chamber with a reflective bottom surface, which is used for reflecting light to measure diffusive light scattering. When an experiment is started, the temperature is decreased in the chamber at a rate of 15 ± 5 °C/min until the detected opacity exceeds a threshold, suggesting that the sample is mostly solid. The system then began to increase the temperature at a rate of 10 ± 0.5 °C/min. Freezing point, or more accurately melting point, is determined when the opacity returns to the original flat line observed while cooling. According to the Phase Technology product brochure, the rated reproducibility is ± 0.8 °C.

In this work, tests are performed on complex fuel samples, single components, and mixtures. The complex fuel mixtures used in this work are all “prescreening fuels” from the FAA ASCENT project 65a. The fuels are sourced from numerous fuel producers, national laboratories, and universities and include many different conversion pathways including hydrothermal liquefaction (HTL), HEFA, and alcohol-to-jet (ATJ). For mixtures, blending was performed by mass and converted to moles, accordingly. Most of the mixtures are using pure components where the molecular weight is provided; for synthetic aromatic kerosene (SAK), the molecular weight is calculated from GC \times GC data.⁹ For the complex fuels, mole concentrations are measured using GC \times GC-MS/FID performed by colleagues at the University of Dayton Research Institute.^{10,11}

3. RESULTS AND DISCUSSION

3.1. Freezing Point Blend Rule Nonlinearity. For many applications, blending rules are desired for the fuel properties. For many properties, a straightforward scalar product between a concentration vector and a property vector is sufficiently accurate for developing synthetic fuel assessments. The freezing point blend rule that was originally adopted by Yang et al.¹² for Tier α fuel prescreening came from the work of Al Mulla et al.³ (presented as the green line in Figure 1), which utilizes a logarithmic transformation but generally mimics a linear by volume blending rule. (Those authors claim a mean absolute error of 0.05 K for this model, but we are skeptical of this value.) The model fundamentally suggests that the addition of species with a higher freezing point than the starting mixture will increase the freezing point and vice versa. This concept strictly competes with the hypothesis of Boehm et al. This model was developed using results from blends of petroleum-based fuels. In petroleum fuels, the freezing component is almost certainly an *n*-alkane that is present in both mixtures. When the component that determines the freezing point is not in both samples, the model falls apart.

Boehm et al. utilized blends of relatively large concentrations (>10%) of high freezing point components (*n*-tridecane and bicyclohexyl) in complex fuels to support the theoretical assertions. These mixtures demonstrated that the fuel into which the freezing component is blended has little effect on the freezing point. However, in these tests, it was known that a high freezing point component was being added to a mixture that was not expected to freeze. This work did not demonstrate

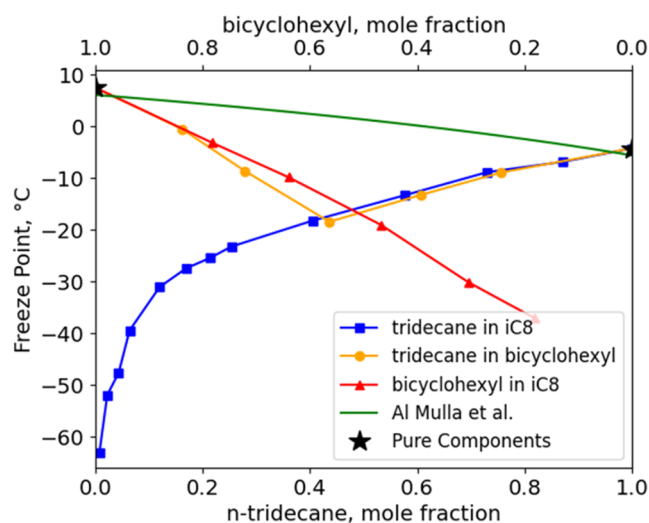


Figure 1. Tridecane and bicyclohexyl blends are measured for freezing point and compared to the old freezing point blend rule. Additionally, “control curves” of bicyclohexyl and tridecane in iso-octane are included to demonstrate that the freezing point of a tridecane limited mixture is the same whether it is blended in a high freezing point substance (bicyclohexyl) or a nonfreezing component (iso-octane).

the assertion that a mixture of two different solutions whose freezing points are controlled by different species can, when blended, result in a mixture with a lower freeze point than either of the preblended solutions. In Figure 1, the freezing points of mixtures of bicyclohexyl in *n*-tridecane (gold line) are compared against the freezing points of bicyclohexyl (red line) and *n*-tridecane (blue line) in a solvent that we know will not freeze, iso-octane (2,2,4-trimethylpentane, freezing point ≈ -110 °C). The freezing points of the neat hydrocarbons used in this work are listed in Table 1. The first observation is the

Table 1. Freezing Points of the Pure Hydrocarbons Used in This Study

name	freezing point, °C
<i>n</i> C8	−58
<i>n</i> C11	−25.5
<i>n</i> C12	−9.5
<i>n</i> C13	−5.3
<i>n</i> C14	5.8
<i>n</i> C15	9.9
<i>n</i> C16	18.1
<i>n</i> C17	21.9
iso-octane	−108
bicyclohexyl	7.5

difference between the green line representing the Al Mulla blending model prediction of the freezing point of the bicyclohexyl/tridecane blends compared to the experimental results of these blends. The freezing point of the blend is consistently lower than the prediction. Now, compare the experimental results of the tridecane/bicyclohexyl blends to the components individually blended in iso-octane. The freezing point of the blends closely tracks the greater of the blue and red lines. There is a bimodal response consistent with the hypothesis of Boehm et al.⁷ This plot emphasizes the issues

with the Al Mulla blending rule and demonstrates the potential for a new method.

3.2. Data-Driven Control Curve Model. *n*-Alkanes are known for their high freezing points and are often blamed when a fuel has a poor freezing point. This is supported by the numerous models correlating *n*-alkane concentration to freezing point.^{2,6} Additionally, *n*-alkanes are typically the highest concentration single species in petroleum-refined fuels. The combination of them being high freezing point species and frequently in relatively high concentrations justifies their selection as species to highlight during fuel screening. They are the focus of this research, but additional species could be included in a similar manner.

Equations 1–3 are the thermodynamically derived equations of Boehm et al.:

$$T_{f,\text{mix}} = \max(T_{f,\text{mix},i}(x_i, i)) \quad (1)$$

$$T_{f,\text{mix},i} = \frac{\Delta H_{\text{fusion},i} + x_i(C_{p,\text{sol},i} - C_{p,\text{liq},i})(T_f - T_{f,\text{mix},i})}{\Delta S_{\text{fusion},i} + x_i(C_{p,\text{sol},i} - C_{p,\text{liq},i}) \ln\left(\frac{T_{f,i}}{T_{f,\text{mix},i}}\right) + \alpha \Delta S_{\text{mixing}}} \quad (2)$$

$$\Delta S_{\text{mixing}} = -\frac{R}{x_j}[(1 - x_j) \ln(1 - x_j) + x_j \ln(x_j)] \quad (3)$$

where T_f is the freezing point temperature, x denotes mole fraction, subscript i denotes various species, H is enthalpy, S is entropy, C_p is heat capacity, and R is the ideal gas constant.

In this work, we suggest the replacement of eqs 2 and 3 with tabulated experimental results of species in a nonfreezing solution (iso-octane). To execute this, we gather data for the freezing point of *n*-alkanes from *n*-undecane (C_{11}) to *n*-heptadecane (C_{17}) in a range of concentrations in iso-octane. The reported lines serve as control curves and represent when the various molar concentrations of these species freeze in a more complex mixture. These control curves are plotted in Figure 2. In Figure 2, it is seen that the freezing point is linear with concentration on a log scale. This feature allows for

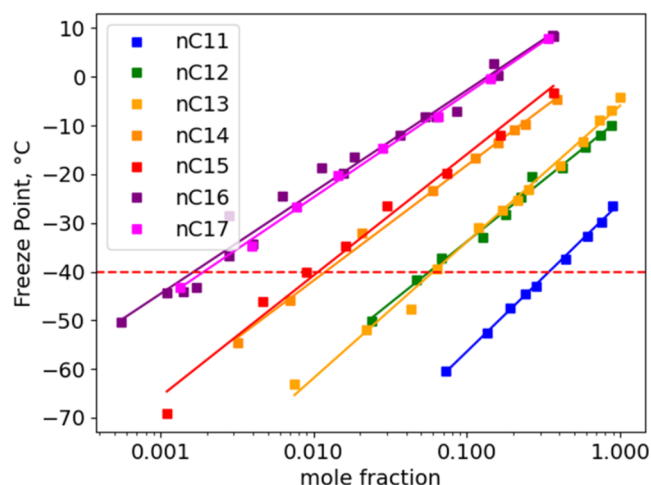


Figure 2. Freezing point of various *n*-alkanes blended in a nonfreezing control solvent (iso-octane). At a given concentration for any of these *n*-alkanes in a fuel, the point at which it will freeze in a fuel can be determined by interpolating the reported data.

interpolation of the best-fit line to determine the freezing point caused by a given species. One noteworthy result from this figure is that at a mole concentration of 0.2% *n*-hexadecane in iso-octane will fail the $-40\text{ }^{\circ}\text{C}$ specification limit for freezing point. This exemplifies why mixtures with *n*-alkanes, especially when associated with higher molecular weight, can have difficulty passing the freezing point; very small quantities of *n*-hexadecane can have a major influence on the freezing point. Another interesting observation is the similarity in the freezing point curves between even/odd pairs of *n*-alkanes (e.g., *n*C14 and *n*C15).

3.3. Freezing Point Prediction Accuracy. The freezing point of 24 sustainable aviation fuel candidates is predicted using the method described above. For consistency, all of the compositional information comes from GC \times GC testing done by the University of Dayton Research Institute. The freezing point values were measured within the laboratory at Washington State University. The sustainable aviation fuel candidates are very diverse, coming from various research pathways. Using the iso-octane control curves from Figure 2 as the prediction, Figure 3 shows the parity plot of the predicted

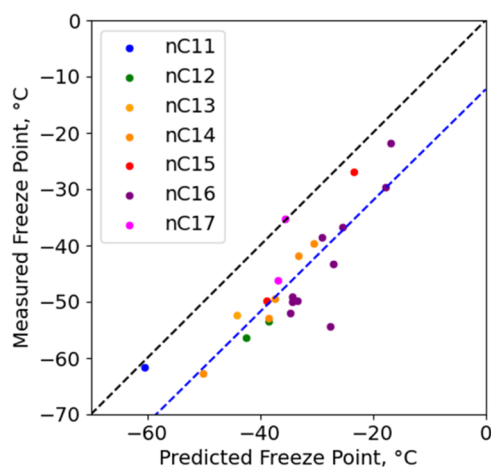


Figure 3. Parity plot of predicted freezing points using the control curve approach compared with measured freezing points. The unity line is included in black, and a best-fit line is included in blue. All of the predictions are higher than the measured freezing points.

and measured freezing points. A step-by-step guide of how to perform these predictions is included in [Supporting Information](#). The unity line is colored black, and the best-fit line is shown in blue. Interestingly, none of the predictions are lower than those in the measurement. This hints that blending with iso-octane represents an upper limit of the freezing point, which is counterintuitive. In these examples, the lower freeze point “solvent” results in a higher freezing point mixture, given the same concentration of the high-freeze-point solute. The predictions generally capture the trend well, but there is a consistent offset of about $12\text{ }^{\circ}\text{C}$. The best-fit line is approximately horizontal to the unity line (slope = 0.988). In addition to the freeze point experimental uncertainty, the greatest potential source of error is the quantification of the *n*-alkane concentrations. This prediction method is sensitive to slight changes in the limiting high-molecular-weight *n*-alkane concentration. There could also be errors associated with the measurement of the control curves, which would propagate into these predictions as well. Moreover, it is entirely possible that the $12\text{ }^{\circ}\text{C}$ offset is not indicative of an error with any of

the model inputs but rather with the assumption that the solvent characteristics such as the number of components, hydrocarbon types, density, or the presence of other solutes that may freeze at nearly the same temperature do not matter. In the next section, we explore this question in more detail.

3.4. Second-Order Effects on the Freezing Point. In Figure 3, we see that the freezing point of a specific species in a mixture is often lower than the freezing point of the same species in iso-octane. Affens et al.¹³ observed that in ternary mixtures of *n*-tridecane, *n*-hexadecane, and Isopar 150 (an isoparaffinic solvent), the freezing point at times decreased when both *n*-hexadecane and *n*-tridecane were present. These results were recreated in our lab using iso-octane in place of Isopar 150 with similar results, albeit to a lesser magnitude. The current results are listed in Figure 4. These results suggest

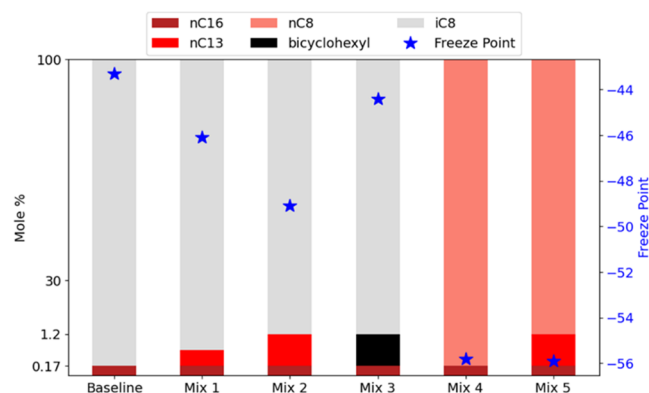


Figure 4. Freezing points of 0.17% hexadecane in various mixtures. Composition is described by the color of the bar. Note: the sizes are not drawn to scale. The freezing point of each mixture is indicated with a blue star. The baseline and mixtures 1 and 2 recreate the results of Affens et al.

that the identity of components other than the first solute to freeze may have some impact on the freezing point of the solute. In this example, normal alkanes and other hexadecane can depress the freezing point of hexadecane, from a 0.17% solution of hexadecane, by up to $12\text{ }^{\circ}\text{C}$, depending on how much of the companion normal alkanes are present. However, the presence of a different solute (bicyclohexyl) that is predicted to freeze out of solution at nearly the same temperature as hexadecane is shown to have little impact on the freezing point of hexadecane.

Returning to the assumptions that fed into the simplified theory that is represented here by eq 2, there are two convenient hypotheses to potentially explain the presence of a second-order effect. One is that the entropy of the mixing term may vary based on the similarity of the solute with the remainder of the solution. The other is that of incomplete separation of molecular species between phases; meaning that perhaps the solid phase is not 100% hexadecane, but rather some solid-state, molecular-level mixture that is mostly hexadecane but partially *n*-tridecane and *n*-octane. Regardless of its cause, the magnitude of this second-order effect seems to plateau at $12\text{ }^{\circ}\text{C}$ for 0.17% hexadecane solutions.

We expanded on this analysis by exploring how different solutions impact the freezing point of the limiting component. Figure 5 shows the freezing point of *n*-hexadecane when blended in various proportions into a variety of solvents. In each case the freezing point of hexadecane is linear with the log

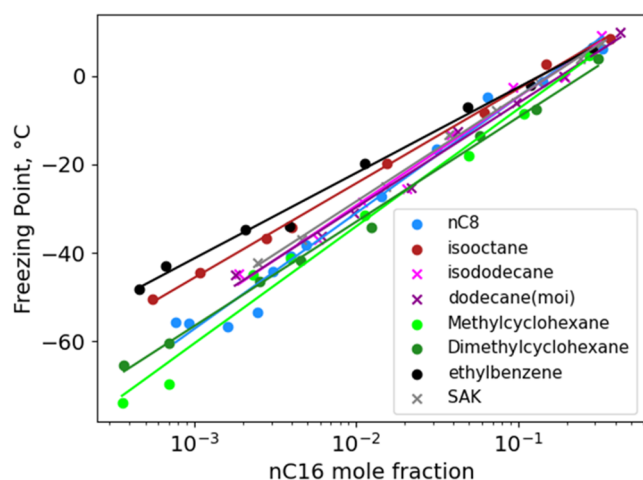


Figure 5. Freezing point of *n*-hexadecane in various solvents. Solvents containing only one species are marked with circles, and mixtures are marked with “x”s. *n*-Alkane and cycloalkane solvents result in a lower freeze point of *n*C16 than aromatic or iso-alkane solvents. The three complex mixtures (two different sets of mixtures of isomers of dodecane and synthetic aromatic ketones (SAK)) all resulted in very similar curves. The “moi” after dodecane stands for “mixture of isomers.”

of its molar concentration. The highest of these curves is what we refer to as the first-order effect, as we assume ethylbenzene has a negligible impact on the purity of the freezing hexadecane and provides a bounding example for the entropy of mixing term (the α scalar) in eq 2. The magnitude of second-order effect is the difference between the top (black, ethylbenzene) curve and any other curve. In this example, methylcyclohexane, dimethylcyclohexane, *n*-octane, SAK, and mixture of dodecane isomers each produce a second-order effect with approximately the same magnitude, which is approximately 30% that of the first-order effect, regardless of the hexadecane (solute) concentration. Pragmatically, the significance here is that both of these effects are always negative. Note: The reference solvent that is chosen to represent the first-order effect may not always be truly bounding; however, there is a significant anecdotal evidence to suggest that complex solvents (such as jet fuels) will never have a less negative second-order effect than any reasonably chosen reference solvent; a single-component hydrocarbon, dissimilar in size and type from the solute.

3.5. 100% *n*-Alkane Fuel. Fuels with large concentrations of *n*-alkanes are generally associated with higher freezing points. Eight of the nine models included in Wang et al.’s review of freezing point included concentration of *n*-alkanes as factors positively correlated with freezing point.² To reinforce one of the critical implications of this method that freezing point is not determined by group concentrations or bulk property characteristics, we created a 100% *n*-alkane fuel with a molecular weight comparable to Jet A with a freezing point below the Jet A specification (-40 °C). This fuel is designed such that every *n*-alkane starting from *n*C16 and descending has approximately the concentration that would cause that species to freeze out in a mixture. The mole concentrations of the fuel blended are included in Table 2. At these concentrations, all of the species between *n*C10 and *n*C16 would be expected to freeze in a solvent at approximately the same temperature (-40 °C). This mixture has an average molecular weight of 145 g/mol and has an ASTM D 2887

Table 2. Mole Percentages Blended for the 100% *n*-Alkane Used Are Given in Figure 6

molecule	mol %
<i>n</i> C16	0.13
<i>n</i> C15	0.91
<i>n</i> C14	0.86
<i>n</i> C13	4.40
<i>n</i> C12	4.57
<i>n</i> C11	25.71
<i>n</i> C10	25.89
<i>n</i> C9	37.52

simulated distillation curve shown in Figure 6. This mixture was designed to emphasize the weaknesses of the empirical

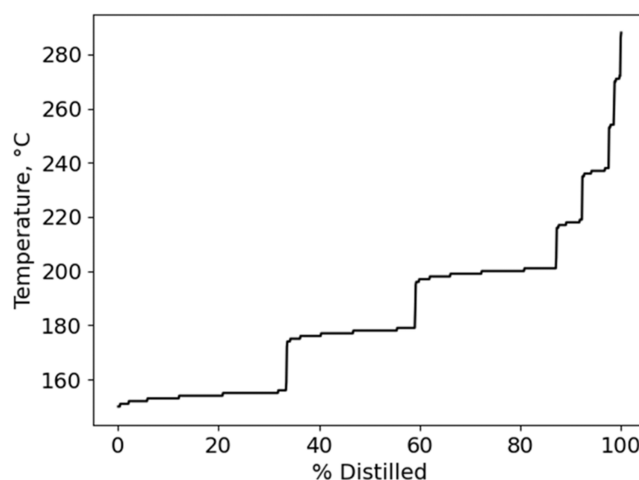


Figure 6. ASTM D 2887 distillation curve of a 100% *n*-alkane fuel.

models based on petroleum-derived samples. Out of the 9 models shared by Wang et al., the closest prediction for the freezing point of this fuel is -12.7 °C; the measured freezing point is -40.7 °C. The model suggested here predicts -44.1 °C. Correlative methods fail to capture the physics which are controlling the freezing point which results in large errors when predicting the freezing point of fuels that are significantly different from those used in creating the model.

4. CONCLUSIONS

Aviation fuel freezing is primarily determined by the freezing point of a single component. Reducing the concentration of that component will lower the freezing point of the mixture, unless another component begins to dominate freezing behavior. To the first order, this phenomenon can be predicted by accurately measuring the concentration of all plausibly limiting solutes in a given sample of an arbitrary hydrocarbon mixture. In petroleum-refined fuels, the limiting species is typically an *n*-alkane. These species are present in high concentrations in petroleum and have high freezing points. Quantities as low as 0.5% of *n*-hexadecane can cause the fuel to be outside of the acceptable freeze point range for jet fuel, regardless of the contents of the remainder of the fuel. For alternative fuels with more diverse and unique compositions, *n*-alkanes will not always be the freeze-controlling species. Many alternative fuel candidates contain high concentrations of single component. For these fuels, the structure of the most prevalent species will be important. Any species that shows up

as a plausible freeze point controlling component can be identified using analytical chemistry approaches, including GC \times GC-VUV. If not already available, this structural isomer identification would be augmented by the creation of new control curves specific to each of the plausible limiting isomers. Once that data is generated, the specific offending species can be identified and targeted for concentration reduction in future synthetic pathways.

Many species in petroleum-refined jet fuel, if isolated, would have a freezing point higher than the $-40\text{ }^{\circ}\text{C}$ limit (for Jet A) set in ASTM D 1655. The same is true of synthetic blend components (SBC). Individually, the SBC must adhere to the requirements detailed in the annexes of ASTM D 7566. The upper limit on the freezing point of SBC is also $-40\text{ }^{\circ}\text{C}$ which is overly restrictive unless the freezing point of the SBC happens to be governed by a high-molecular weight, normal alkane, which is not the case for any of the eight synthetic pathways approved thus far. The results of this work suggest that the freezing point of all SBC/petroleum blends will be less than the freezing point of either one prior to mixing and that the limit for SBC should be applicable to a blend of the SBC at its maximum allowed concentration with some reference solvent. However, a note of caution should be added, stating that a higher freezing point may be observed for SBC/petroleum blends if the petroleum component happens to contain a significant concentration of the same molecule that is controlling the freezing point of the neat SBC. Ultimately, the freezing point limit that is specified in ASTM D 7566 (Table 1) shall control the SBC/petroleum blend.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.energyfuels.4c06091>.

Freezing point prediction process; graphical solution to the prediction of freezing point using the method proposed in this paper (PDF)

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Notes

The authors declare no competing financial interest.

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