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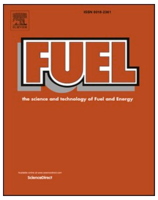

Full Length Article

Assessing the effect of composition on dielectric constant of sustainable aviation fuel

Zhibin Yang [a,*], David C. Bell [a], Randall C. Boehm [a], Pedro Fischer Marques [b], Jessica A. Boze [b], Ilya V. Kosilkin [b], Joshua S. Heyne [a,c]

[a] *Bioproduct, Sciences, and Engineering Laboratory, School of Engineering and Applied Science, Washington State University, Richland, WA 99354, USA*
[b] *The Boeing Company, BCA Propulsion Systems Engineering, Everett, WA 98204, USA*
[c] *Energy Processes and Materials Division, Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, WA 99352, USA*

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ABSTRACT

One of the challenges in developing 100% sustainable aviation fuels is the effect of synthetic blend components on the dielectric constant. Modern aircraft often employ capacitance-based gauging systems that rely on the dielectric constant of the fuel onboard to determine fuel quantity. Aircraft manufacturers have expressed concern over inaccuracies in fuel gauging attributable to variances in the dielectric constant between conventional jet fuels and 100% paraffinic sustainable aviation fuel. In our study, dielectric constant and density data were gathered from 172 conventional jet fuel samples to establish a baseline "experience range." Subsequently, thirty-five individual hydrocarbon molecules from the jet fuel range and nine fuels were acquired, characterized, and reported herein according to the Clausius-Mossotti relationship. Our findings indicate that different hydrocarbon group types exert varying effects on the Clausius-Mossotti relationship. To align with the established experience range for both the dielectric constant and the Clausius-Mossotti relationship, it appears that 100% drop-in SAF will need to incorporate some aromatic compounds. Finally, we explored two blending rules for the dielectric constant of jet fuel range hydrocarbons and achieved excellent coefficients of determination (R^2 values of 0.9942 and 0.9983, respectively).

1. Introduction

Commercial aviation is one of the safest means of travel. This is due to a combination of industry regulations, rigorous pilot training, and redundancy of aircraft components. Safety is and always will be paramount on commercial airlines and at the forefront of development efforts toward commercial airlines' net-zero 2050 carbon emission goals [1]. Sustainable aviation fuel (SAF) is the key contributor to this goal. Other technologies have been envisioned, including hydrogen and electrification. However, the technology readiness level of these technologies are low, rendering them unlikely to contribute as much as SAF toward the carbon emissions goal by 2050 [2–4].

Several currently approved synthetic blending component pathways in ASTM D7566-22 are allowed to be blended up to 50 % by volume (A3 and A7 are limited to 10 % by volume) with conventional jet fuel for commercial usage. The blend limits of these various annexes are due to differences in fuel properties outside of the petroleum experience, such as density and material compatibility (i.e., O-ring seal swell). Another concern raised by aircraft manufacturers is possible inaccuracy in fuel gauging due to the difference in the relationship between density, dielectric constant and temperature for jet fuels derived from synthetic sources (i.e., 100 % paraffinic SAF) when compared to jet fuels from crude oil. With the diversification of SAF feedstocks, conversion processes, and product compositions, there remains significant uncertainty in regard to the impact all this has on the dielectric constant and other properties. As per ASTM D4054, dielectric constant and many other properties are considered "fit-for-purpose" properties, which are not controlled explicitly by the fuel specifications (ASTM D1655, UK MoD Def Stan 91–091, ASTM D7566, MIL-DTL-83133, MIL-DTL-5624, etc.). Despite not being explicitly regulated, these properties are vital for engine and airframe fuel system design and undergo assessment during the ASTM D4054 approval process.

Precise fuel quantification aboard aircraft is essential for ensuring operational safety and efficiency. Fuel quantity indicating systems (FQIS) on contemporary aircraft, typically employ capacitance or speed of sound methods to gauge fuel levels, with the former being more

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* Corresponding author.
E-mail address: zhibin.yang@wsu.edu (Z. Yang).

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widespread. These systems are influenced by fuel characteristics, with capacitance-based FQIS leveraging the Clausius-Mossotti relationship to correlate the measured dielectric constant with fuel density. Consequently, fuel mass, rather than volume — which can fluctuate with temperature changes experienced during flight — is utilized to ascertain the aircraft's operational range. The system computes the on-board fuel mass by combining volume measurements with density calculations, derived from capacitance readings. While some aircraft enhance FQIS accuracy with onboard densitometers for direct density measurement, this feature is not universal.

Capacitance based FQIS gauging relies on the following major parameters: dielectric constant, voltage, frequency, and geometry. The latter three are fixed in the aircraft design, so the only variable parameter is the dielectric constant. The dielectric constant (i.e., relative permittivity) is a function of the fuel composition and temperature. The major aircraft manufacturers use some combination of historical data to design their FQIS. In practice, deviation from the hard-coded Clausius-Mossotti line will cause either an over or under-estimation of fuel on board. A fuel gauging error of ± 6 % is typical [5], supposing that the dielectric constant is treated as a constant independent of temperature and fuel type. By introducing dielectric compensation, this error is reduced to ± 2.5 % [5], where the compensator is typically located at the bottom of the fuel tank. Most aircraft have a densitometer installed, but the industry is now increasingly using the densitometer only on the ground due to air bubbles (outgassing), vibrations in-flight, etc. Where the dielectric constant, density, and temperature of the uplifted fuel during refueling are measured and then mapped to dielectric and temperature sensors in all tanks, density can also be inferred using the Clausius-Mossotti relationship, which contributes about ± 1.2 % [5] to overall accuracy error.

The two latest world fuel surveys of performance and fit-for-purpose properties for aviation jet fuels include ARINC 611 [6] and CRC 647 [7]. A total of 172 jet fuel samples from around the world were collected and characterized, generating a total of 1200 data points on density and dielectric constant. This data was used to correlate density and dielectric constant using the Clausius-Mossotti relationship. Relatively similar slopes and intercepts are observed for both data sets. While both of these surveys are excellent, it should be recognized that 172 samples are a small fraction of the total population. This data is suitable for highlighting trends and average values; however, the relatively modest data set does not accurately define the distribution's shape and should not be used to deduce the range's extreme property values.

Unlike other properties that are mentioned in ASTM D4054, the dielectric constant of aviation fuel is largely unstudied. Sen et al. [8] were able to observe that dielectric constants of mixtures of liquid hydrocarbons exhibited linear relationships with volume fraction by investigating light alkanes (C2-C7) and some hydrocarbon mixtures using a slotted line technique at 1.2 GHz and at atmospheric pressure over a temperature range of 115–295 K. Pan et al. [9] explored the dielectric constant and Clausius-Mossotti functions for liquid mixtures containing nitrogen, argon, and light hydrocarbons. The liquefied natural gas densities were determined from accurately measured dielectric constants and compositions. Sharma et al. [10] studied the measurement of dielectric parameters of aviation fuel at various frequencies using the cavity perturbation technique, which showed that the dielectric constant of jet fuel is a function of frequency at X-band frequencies. Brazier et al. [11] studied the effect of pressure on the density, viscosity, and dielectric constant of some light hydrocarbons. While there is some published research on the dielectric constant of hydrocarbons, there are no published studies on the effect of synthetic blend components or sustainable aviation fuel or jet fuel composition on the dielectric constant and the Clausius-Mossotti relationship.

Here, we report the dielectric constant and density measurement for four conventional fuels, thirty-four neat jet fuel range hydrocarbons, thirty-two mixtures, and six synthetic blending components (SBC) over a range of 10 to 30 °C. One hundred and seventy-two different jet fuel dielectric constant and density measurements over the range of −35 to 70 °C were gathered from two reports to establish a conventional jet fuel experience range. These new data are used to investigate the effect of SAF on the dielectric constant and evaluate two different blending rules for dielectric constant estimation of jet-range hydrocarbon mixtures, while the mined data is used to characterize the conventional fuels experience range.

2. Materials and methods

a) Reference materials

Forty-five hydrocarbon materials were sourced from five vendors and six fuel producers. The details of these materials are included in Table 1.

b) Density and dielectric constant measurement

The Stanhope-Seta equipment, JetDC, was used to measure both density and dielectric constant according to IP 638 [12]. The JetDC has a density range from 0 to 900 kg/m^3, a dielectric constant range from 1 to 2.5, and a temperature range from 10 to 30 °C with a temperature resolution of 0.01 °C. An existing standard test method (ASTM D924) for relative permittivity for electrical insulating liquids provides a procedure for measurements at frequencies between 45 and 65 Hz. This is a different frequency than is used for the equipment installed on airplanes, and these lower frequencies have significant interference from water. Thus, the new JetDC (5000 Hz) was designed for conventional jet fuel and SAF.

A brief description of the standard test method follows. the sample is loaded into the cell at 20 °C, the cell is cooled to 10 °C and the density and dielectric constant are measured, the cell is then warmed up in 5 °C increments up to 30 °C, and at each new temperature the density and dielectric constant are measured.

The permittivity measurement cell consisted of an inner, outer, and guard electrodes with a known cell constant. The capacitance is measured at each temperature at an excitation frequency of 5000 Hz. The density measurement utilized a resonance-type measurement with an accuracy of 0.5 kg/m^3. The relative permittivity (ε_r) is calculated using Equation (1).

$$\boldsymbol{\varepsilon_r} = \boldsymbol{C_s}/\boldsymbol{C}_0 \tag{1}$$

In Equation (1), C_s is the capacitance of the test cell containing the sample and C_0 is the capacitance of the test cell under vacuum. Obtaining a vacuum can be problematic and a more practical means to obtain the cell constant is to use a certified reference material in which case Equation (2) is used to calculate C_0.

$$\boldsymbol{C}_0 = \boldsymbol{C_{cyclohexane}}/\boldsymbol{\varepsilon_{rcyclohexane}} \tag{2}$$

Where $C_{cyclohexane}$ is the capacitance of the cell containing certified reference cyclohexane, and $\varepsilon_{rcyclohexane}$ is the certified value for relative permittivity of the certified reference cyclohexane.

c) Clausius-Mossotti relationship

Two forms of the Clausius-Mossotti relationship are represented in Equations (3) [13] and (4) [5], respectively. In these equations, the dielectric constant at a given temperature (dimensionless) is denoted by $\boldsymbol{\varepsilon_r}$, the molecular weight of the fuel (g/mol) is denoted by MW, the molar polarizability (cm^3/mol) is denoted by R, and the fuel density at a given temperature (g/cm^3) is denoted by $\boldsymbol{\rho}$. For jet fuel, the published values [5] for the constants A and B are 1.0 ± 10 % and 0.3658, respectively.

$$\frac{\boldsymbol{\varepsilon_r} - 1}{\boldsymbol{\varepsilon_r} + 2} = \frac{\boldsymbol{\rho R}}{\boldsymbol{MW}} \tag{3}$$

Table 1
The hydrocarbons used in this study, including the source and purity.

Name	Type	Supplier	Purity
hexane	*n*-alkane	Sigma-Aldrich	>99 %
heptane	*n*-alkane	ACROS	99 %
octane	*n*-alkane	ACROS	99 %
nonane	*n*-alkane	ACROS	99 %
decane	*n*-alkane	Thermo Scientific	99 %
undecane	*n*-alkane	Thermo Scientific	99 %
dodecane	*n*-alkane	Thermo Scientific	99 %
tridecane	*n*-alkane	TCI	>99 %
tetradecane	*n*-alkane	Thermo Scientific	>99 %
2,3-dimethylbutane	*iso*-alkane	Thermo Scientific	>98 %
2,2,4-trimethylpentane	*iso*-alkane	Thermo Scientific	99 %
2,6,10-trimethyldodecane	Synthetic paraffinic kerosene (SPK)	Amyris	N/A
2,2,4,4,6,8,8-heptamethylnonane	*iso*-alkane	Thermo Scientific	98 %
cyclohexane	cycloalkane	Thermo Scientific	99 %
methylcyclohexane	cycloalkane	Thermo Scientific	99 %
cycloheptane	cycloalkane	TCI	99 %
cyclooctane	cycloalkane	Thermo Scientific	>99 %
ethylcyclohexane	cycloalkane	ACROS	>99 %
1,2-diethylcyclohexane	cycloalkane	TCI	98 %
1,2,4-trimethylcyclohexane	cycloalkane	TCI	>96 %
tert-butylcyclohexane	cycloalkane	Thermo Scientific	>99 %
1,4-dimethylcyclooctane (DMCO)	Cyclo paraffinic kerosene (CPK)	CleanJoule, Mukund Karanjikar	N/A
trans-decalin	cycloalkane	TCI	>98 %
cis-decalin	cycloalkane	TCI	98 %
bicyclohexyl	cycloalkane	TCI	>99 %
toluene	aromatic	Thermo Scientific	99 %
ethylbenzene	aromatic	Thermo Scientific	99 %
n-propylbenzene	aromatic	Thermo Scientific	98 %
m-xylene	aromatic	TCI	>99 %
o-xylene	aromatic	TCI	98 %
p-xylene	aromatic	Thermo Scientific	99 %
n-hexylbenzene	aromatic	Alfa Aesar	98 %
1,2,3-trimethylbenzene	aromatic	Sigma-Aldrich	>89 %
1,2,4-trimethylbenzene	aromatic	TCI	>98 %
1,3,5-trimethylbenzene	aromatic	TCI	>97 %
1-methylnaphthalene	aromatic	Thermo Scientific	96 %
tetralin	aromatic	Thermo Scientific	97 %
n-butylbenzene	aromatic	Thermo Scientific	>99 %
A-1 (POSF 10264)	Jet A	AFRL, Tim Edwards	N/A
A-2 (POSF 10325)	Jet A	AFRL, Tim Edwards	N/A
A-3 (POSF 10289)	Jet A	AFRL, Tim Edwards	N/A
Hydroprocessed Esters And Fatty Acids (HEFA)	SPK	World Energy	N/A
Fischer-Tropsch Synthesized Paraffinic Kerosine (FT-SPK)	SPK	AFRL, Tim Edwards	N/A
Synthetic Aromatic Kerosene (SAK)	SAK	Virent	N/A
Alcohol-To-Jet Synthetic Paraffinic Kerosene (ATJ)	SPK	AFRL, Tim Edwards	N/A
Cycloparaffinic Kerosene (CPK0)	CPK	Shell	N/A
JP-10	Jet Fuel	AFRL, Tim Edwards	N/A

$$\frac{\boldsymbol{\varepsilon_r} - 1}{\boldsymbol{\rho}} = \boldsymbol{A} + \boldsymbol{B}(\boldsymbol{\varepsilon_r} - 1) \tag{4}$$

While Equation (3) is true only for materials with no permanent dipole moment, it may be particularly useful for the prediction of dielectric constant for conceptualized fuels or even neat hydrocarbons because polarizability, density, and molecular weight are each readily predictable or well documented. Equation (4) is generally true, but the constants are dependent on the material and heretofore have been determined empirically, via linear regression, by collecting density and dielectric constant data over a series of temperatures. By ignoring the material dependence of A and B and rearranging Equation (4) to Equation (5), the density of fuel is estimated from its measured dielectric constant. A prominent goal of this research is to inform the aviation research community of the implication of ignoring the material dependence of A and B as the composition of (potential) future jet fuels deviates from the composition of fuels used to generate the reference database that was used to establish the constants, A and B for jet fuel.

$$\boldsymbol{\rho} = \frac{(\boldsymbol{\varepsilon_r} - 1)}{\{\boldsymbol{A} + \boldsymbol{B}(\boldsymbol{\varepsilon_r} - 1)\}} \tag{5}$$

d) Reference database for conventional jet fuels

Per ASTM D4054, the dielectric constant is considered a fit-for-purpose property. It is not controlled explicitly by the fuel specifications but is important for capacitance-based FQIS gauging. As such, it is important to establish the experience range of Clausius-Mossotti plot data for conventional jet fuel. Combined, the datasets from ARINC 611 and CRC 647 account for 1200 data points from 172 different Jet A fuel samples. The ARINC data was taken at −35 to 25 °C at 10 °C increments and the CRC data was taken at various temperature increments from −35 to 70 °C. The Clausius-Mossotti plot is generated for each of the 172 fuel samples to derive a conventional jet fuel experience range for both the slope and intercept. It should be noted that the ARINC data was published in 1999 and the CRC was published in 2006. It is certainly possible that modern Jet A fuel has lower aromatic content and lower cycloalkane content due to industry-wide changes in petroleum refining practices [14]. However, any year-over-year trend in the average composition of jet fuel is believed to be small relative to the worldwide variation in jet fuel composition observed over any 12-month period since records of jet fuel composition have been kept.

e) Blending rule for mixture

Predicting the dielectric constant of fuel blends is particularly valuable, given the impracticality of conducting dielectric constant measurements for every individual blend ratio. Two blending rules were evaluated against measurement. One predicts the mixture's dielectric constant directly from the component volume fraction and dielectric constant, and the other predicts the mixture's dielectric constant from the mixture polarizability and molar volume. The volume fraction blending rule, expressed here as Equation (6), was first introduced by Sen et al. [8] for light alkanes (C2-C7). We apply it here to liquids because the dielectric constant is linear with density, and density has a volume fraction blending rule. In this equation, $\boldsymbol{\varepsilon_{rmix}}$ denotes the dielectric constant of the mixture and v_i and ε_{ri} are the volume fraction and neat dielectric constant, respectively of the i$^{\text{th}}$ component. The advantage of this blending rule is that no additional information regarding the mixture is required to do the calculation.

$$\boldsymbol{\varepsilon}_{rmix} = \sum \boldsymbol{v}_i{}^*\boldsymbol{\varepsilon}_{ri} \tag{6}$$

For nonmagnetic materials with no permanent dipole, the dielectric constant, ε_r is related to the polarizability (R) by a simple algebraic expression written here as equation (7). The blending rule for polarizability, expressed here as Equation (8), has been widely disseminated [15] and is extraordinarily accurate. Moreover, the polarizability of saturated hydrocarbons can be predicted with excellent accuracy via a group additivity approach [16]. The accuracy of such models applied to aromatic hydrocarbons is not well understood, and thus the 'effective polarizability' (defined as the result of Equation (7)) of aromatic species in fuel may require substantially more intricate models or determination from measured density and dielectric constant. Once the polarizability of the mixture is determined from Equation (8), it is straightforward to rearrange Equation (7) to calculate the dielectric constant or the molar volume of the mixture provided the other is known. It cannot be used to simultaneously predict both density and dielectric constant. In other words, this analysis is ideal for mixtures with well-known composition, from which molar volume can be readily determined. However, for commercial fuel, which is a complex mixture with incomplete composition illumination, a more direct approach for estimating the dielectric constant of a mixture of fuels, such as Equation (6), is preferred.

$$\boldsymbol{R} = \boldsymbol{V}_m{}^*\frac{\varepsilon_r - 1}{\varepsilon_r + 2} \tag{7}$$

$$\mathbf{R}_{mix} = \sum \boldsymbol{v}_i{}^*\boldsymbol{R}_i \tag{8}$$

3. Results and discussion

A Clausius-Mossotti plot is provided in Fig. 1, showing all 1200 data points (open circles) from the database described in the abovementioned section and the best-fit line (dash lines) through these points. The slope and intercept of the combined data are 0.35944 and 1.0005, respectively, which is consistent with the published value [5] for constant A is 1.0 ± 10 %, and constant B is 0.3658. Since the dielectric constant varies inversely with temperature, the lower-left of this plot is populated by the higher-temperature portion of the CRC dataset and is not a reflection of any fuel composition differences between the two datasets. The cluster of 18 blue points below the trend line originates from three fuel samples drawn from different places around the world. All three samples have a lower aromatic content (14.1 v%) compared to the CRC average (20.0 v%) and elevated total cycloalkanes content (42.5 v%), especially in dicycloalkanes content (23. 5v%) compared to CRC average of 21.1 v% and 9.0 v%, respectively. It is worth noting that the lowest aromatic sample is a 100 % synthetic fuel from South Africa with 5.6 v% aromatic content and a 2.6 v% total cycloalkanes content. However, this fuel has a dielectric constant that is well within the conventional fuel range. The technical reason behind this observation will be discussed in a later section. The linearity of dielectric constant with respect to temperature for jet fuel in the liquid range is also investigated, where the temperature range is restricted (−35 to 25 °C for ARINC data and −35 to 70 °C CRC data) to avoid highly non-linear features that present in many properties as the temperature approaches a phase transition (freezing or boiling). The average R-square value for the 172 dielectric constant versus temperature correlations is exceptional, 0.99989.

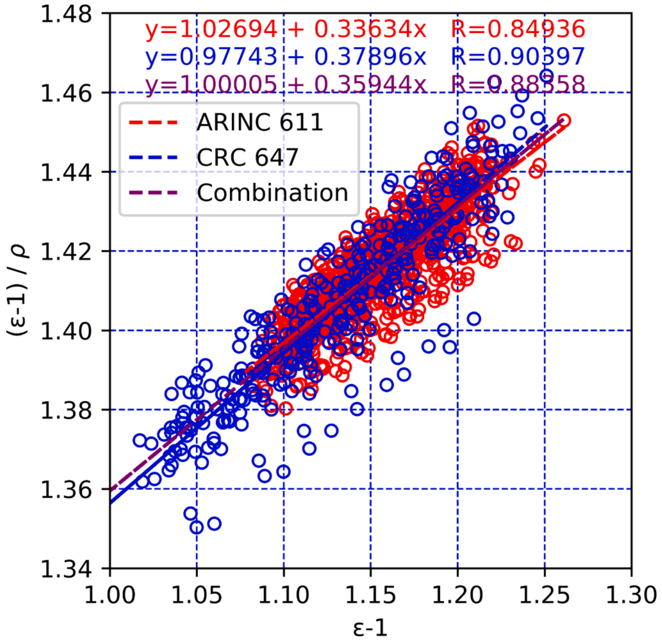

Fig. 1. Clausius-Mossotti relationship for 172 different jet fuel samples. The dielectric constant and density of 114 Jet A sample at −35 to 25 °C are from ARINC report (red open circles), and dielectric constant and density of 57 Jet A sample at −35 to 70 °C are from CRC report (blue open circles). In addition, the best fit line of ARINC data (red dash line), CRC data (blue dash line), and the combination of both report (purple dash line) are also reported.

It is understood that different hydrocarbon types (normal, iso, cycloparaffins, aromatics, diaromatics) have different dielectric properties (absolute values at a given temperature and slopes of dielectrics vs. density relationship) [17]. The typical distribution of hydrocarbons that were historically present in turbine fuels (e.g., aromatic content around 16–18 v%), resulted in a combination of dielectric values that aviation industry and fuel probe manufacturers accepted as typical for design and calibration of fuel quantity indication systems. Most modern aircraft rely on these properties for the accurate gauging of fuel on board.

Fuels with unique distribution of hydrocarbons such as those that lack of an entire hydrocarbon type, aromatics or cycloparaffins will have dielectric properties that are outside of the typical experience (e.g., absolute value and/or slope). Use of such fuels in fuel systems that rely on an average hardcoded relationship of dielectric permittivity vs. density will result in inaccurate estimation of fuel quantity.

Due to the nature of the production process fuels from unconventional sources often lack one or more type of hydrocarbons. For example, HEFA SPK predominantly consists of *iso*-paraffins, virtually no aromatics, and has a relatively low proportion of cycloparaffins. As a result, dielectric properties of emerging fuels (SAF) are likely going to be outside of the current typical experience. Better understanding of how chemistry of emerging fuels impacts dielectric properties is needed.

Since it is virtually impossible to find fuels with properties near the outer corners of the experience range, selected single molecules and simple mixtures are used to represent the corners of the real fuel experience range. Single molecule hydrocarbons that represent major hydrocarbon types found in turbine fuels were chosen for this study. These included n-paraffins, *iso*-paraffins, cycloparaffins, and aromatics. Each type is represented by different substitution patterns, providing insight into the structure – dielectric property relationship.

To better understand the different hydrocarbon type effects on the Clausius-Mossotti relationship, data from the thirty-four individual hydrocarbon molecules and nine fuels (10 to 30 °C) are plotted in Fig. 2, where the 172 reference jet fuels were also extrapolated/interpolated to 10 to 30 °C to create a back-to-back comparison. In general, the saturated hydrocarbons were clustered at the bottom left of Fig. 2, where n- and *iso*-alkanes were mostly on the same line as the reference fuels but at a lower density. This is no surprise since n- and *iso*-alkanes makes up most of the jet fuel composition. The cycloalkanes fall below the reference fuel line, while the polycycloalkanes are positioned farther away from it. The dielectric constant of cycloalkanes, n-alkanes and *iso*-alkanes are similar. The reason that cycloalkanes deviate from the trendline is because of the difference in density at a given temperature.

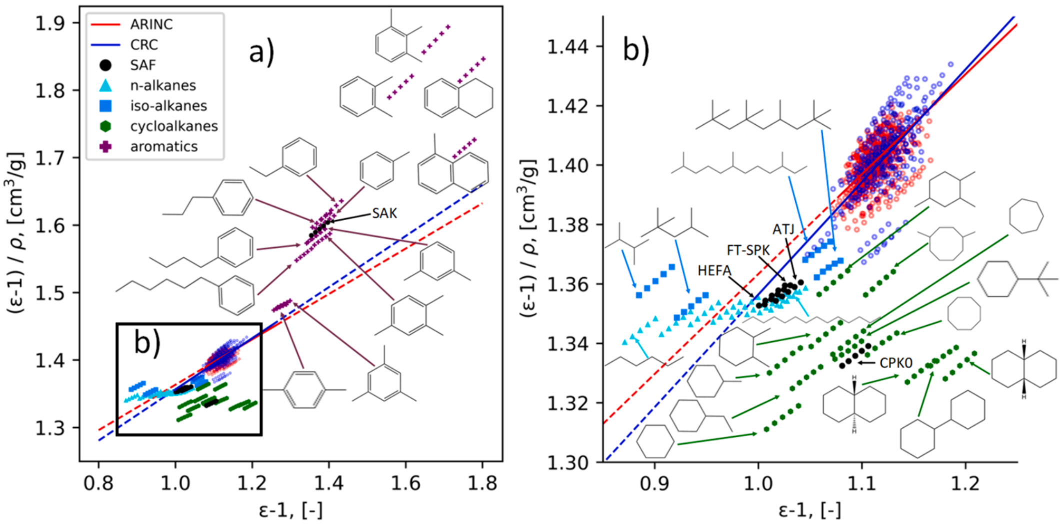

Fig. 2. Clausius-Mossotti relationship of neat hydrocarbons that are in the jet fuel range. All 172 reference Jet A were interpolated/extrapolated to 10 to 30 °C to compare with the measurement done on JetDC. The neat molecule's structure was also presented next to the data point for better illustration.

The unsaturated hydrocarbons, or aromatics, are on the top right corner of the Clasusius-Mossotti plot. It is observed that all three 100 % paraffinic SAFs (HEFA, FT-SPK, and ATJ) exhibit similar dielectric constants and Clausius-Mossotti relationship. This finding is consistent with expectations, given that these SAFs consist entirely of normal and branched alkanes. Contrastingly, SAK is primarily composed of mono-aromatic compounds [16]. This chemical composition accounts for its proximity to other mono-aromatic fuels on the Clausius-Mossotti plot. Note the large difference between the dielectric properties of o-xylene and p-xylene. This interesting observation is discussed in a later section.

To further assess the variation in fuel samples and hydrocarbon type, the constants of the Clausius-Mossotti relationship were computed for each temperature series of each fuel sample, and these values are shown in Fig. 3. The locus of points corresponding to petroleum fuels resides along a straight line. Linear extrapolation of this line to a lower slope (higher intercept) brings it into the data corresponding to all neat iso and normal alkanes (nC6 to nC14) provided in Table 1. Most of the data corresponding to cycloalkanes resides to the left (or below) this line, while most of the data corresponding to unsaturated hydrocarbons resides to the right (or above) this line. Such a feature-level difference between different hydrocarbon types raises concern that future fuels, with markedly different compositional characteristics relative to conventional fuels, may require software (or gauging) changes to aircraft systems used to determine fuel quantity. The purpose of Fig. 3 is not to compare pure aromatics with conventional jet fuel but to see the effect of the hydrocarbon group type on the Clausius-Mossotti relationship.

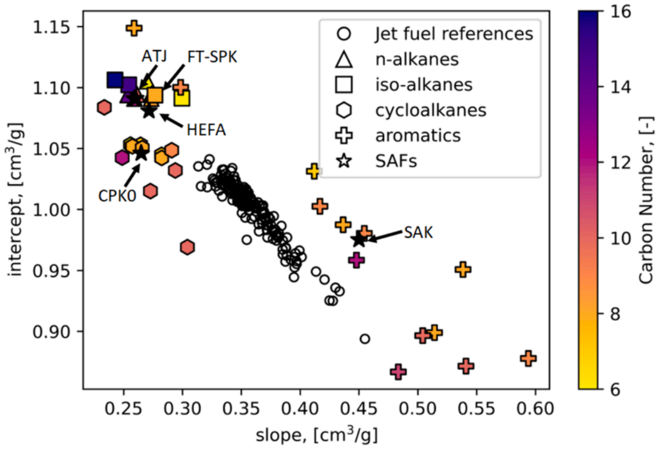

Fig. 3. The slope and intercept of all 172 Jet A (black open circles) and neat molecules (solid-colored circles). A color gradient also presents the carbon number associated with individual molecules.

Since the Clausius-Mossotti relationship is an algebraic manipulation of density, and dielectric constant, there is merit in investigating each property independently. Fig. 4 illustrates the density (a) and dielectric constant (b) slope and intercept as a function of temperature. While the three different isometric variances of xylene have similar densities, their dielectric constants vary considerably. One interesting observation that could be made is that the conventional fuel density range could be met with just n- and *iso*-alkanes and cycloalkanes; no aromatic would be needed. In the SAF community, it is of great interest to use cycloalkanes to replace aromatic to satisfy the density and material compatibility (e.g., seal swell) requirement while reducing the sooting propensity of the blended fuel.

The slope from the Clausius-Mossotti plot strongly correlates with the molecule's permanent dipole moment, as shown in Table 2. The correlation coefficient of the slope of the dielectric constant and permanent dipole moment on selected aromatics is 0.89. This explains why the saturated compounds were all clustered in the bottom right of the Fig. 4(b). This also explains the large difference between o-xylene and p-xylene in the Clausius-Mossotti plot. Upon examination of Fig. 4 it becomes clear that some amount of aromatics is required in a mixture in order to match the dielectric properties range of conventional jet fuel. Since both n- and *iso*-alkanes and cycloalkanes are on the bottom right of the conventional fuel in Fig. 2, some of the top left aromatic points will be needed to bring the blended fuel into the conventional fuel range.

Being able to accurately predict the dielectric constant of blends of two fuels is also of significant interest since dielectric constant measurement on every single blend ratio is not feasible. The Clausius-Mossotti relationship can be predicted before any blending occurs. In light of this, the accuracy of the two abovementioned blending rules were investigated against 24 neat molecules and fuels at various blend ratios, which include 40 mixtures and 200 data points. The mixtures consist of neat molecule to neat molecules, neat molecules to fuel, and fuel to fuel blending. For detailed information regarding neat molecules, mixture blend ratio, etc., please refer to the supplemental information.

Both the volume fraction and polarizability blending rules achieved excellent results. Fig. 5 shows the dielectric constant measurement versus prediction for both volume fraction (green open circles) and polarizability (red x markers) blending rules. The predicted points

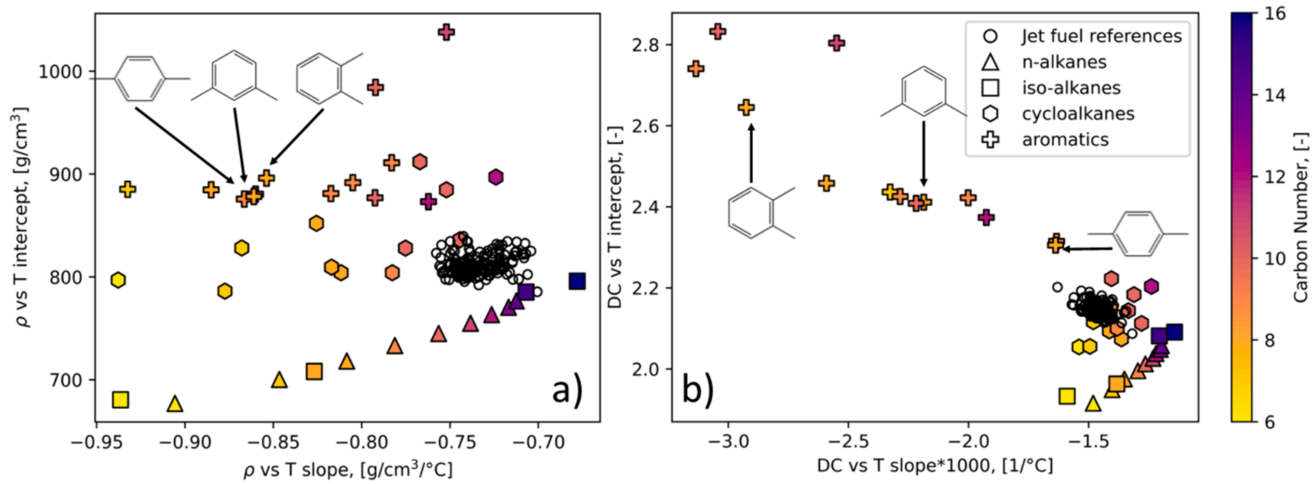

Fig. 4. Density (a) and dielectric constant (b) slope and intercept as a function of temperature, the open black circles are the reference jet fuels. Some of the aromatics molecule's structure was presented next to the data point for better illustration. A color gradient also presents the carbon number associated with individual molecules.

Table 2
The slope of dielectric constant with respect to temperature and permanent dipole moment of selected aromatics. The permanent dipole moment of aromatic compounds are taken from the work of Zhao et al. [18].

Molecules	DC slope*1000, [°C]	Permanent dipole moment, [D]
1,2,3-trimethylbenzene	−3.1346	0.660
o-xylene	−2.9254	0.582
toluene	−2.3262	0.343
1-methylnaphalene	−2.5492	0.318
ethylbenzene	−2.5912	0.297
1,2,4-trimethylbenzene	−2.0012	0.291
m-xylene	−2.1864	0.271
p-xylene	−1.6376	0.081
1,3,5-trimethylbenzene	−1.6336	0.047

corresponding to the volume fraction blending rule employed only the neat molecules/fuels' dielectric constant; no other information is required by this model. The volume fraction blending rule achieved a mean absolute error (MAE) of 0.0038, mean standard error (MSE) of 0.000039, mean error (ME) of 0.0037, and R-squared of 0.9942. For the predictions corresponding to the polarizability blending rule, neat component data, including dielectric constant, density, and MW, were employed to determine the fuel polarizability and molar volume, respectively. The polarizability blend rule achieved a MAE of 0.002, MSE of 0.000011, ME of 0.0004, and R-squared of 0.9983. As seen visually and numerically in Fig. 5, MAE and ME values are nearly equal to one another. The volume fraction blending rule appears to result in a small bias higher than the measured data.

Aromatics are needed for 100 % drop-in capacitance based FQIS compatibility. The fuel community has demonstrated a strong interest in the development of 100 % drop-in SAF options while simultaneously aiming to reduce or eliminate aromatics in these fuels to address particulate matter emissions. In recent years, many publications have illustrated the ability of cycloalkanes to complement SPKs [19], e.g., density, material compatibility [20], while lowering the sooting potential of the fuel [21,22]. In contrast to those previous studies, cycloalkanes do not complement n- and *iso*-alkanes. Instead, here they adversely affect the Clausius-Mossotti relationship. Meaning, replacing aromatics with cycloalkanes is not an option for this property. The precise quantity and type of aromatics required remains unclear at this stage for 100 % drop-in capacitance based FQIS compatibility. Furthermore, mono-aromatic compounds, such as those found in SAK, can offer enhanced dielectric constant to most 100 % paraffinic SAF pathways, while simultaneously reducing overall particulate matter emissions when compared to traditional jet fuels [16].

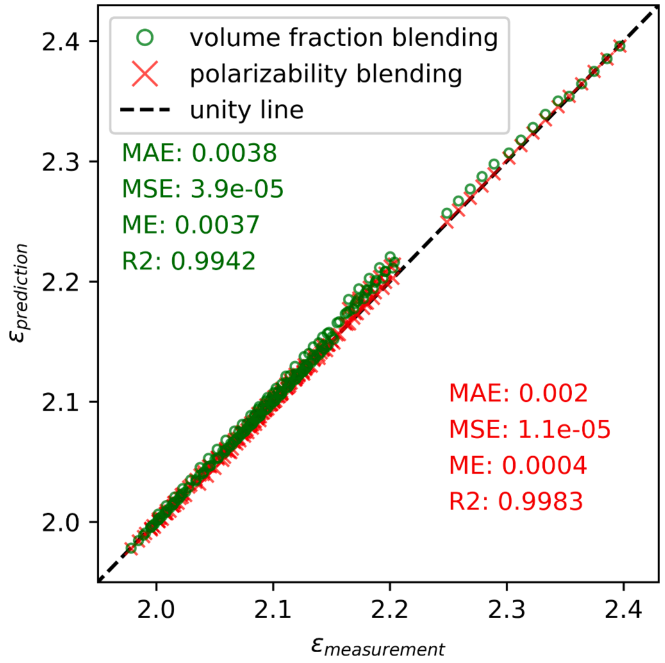

Fig. 5. Prediction versus measurement of the dielectric constant of volume fraction (green open circles) and polarizability (red x) blending rules. The black dashed line represents the unity line.

4. Conclusion

In this study, we presented the Clausius-Mossotti relationship experience based dielectric permittivity measurements of 172 worldwide conventional jet fuels. Additionally, the effect of hydrocarbon types (studied as pure single molecule compounds) and substitution pattern on the dielectric constant and subsequent Clausius-Mossotti relationship was investigated. We showed that the permanent dipole moment of jet fuel range hydrocarbons has a strong correlation with the orthogonal distance away from the Clausius-Mossotti relationship commonly accepted in modern capacitance-based FQIS. We conclude that to reach the current jet fuel experience range for both the dielectric constant and the Clausius-Mossotti relationship, SAF made from 100 % paraffins will most likely require a minimal concentration of aromatics in order to avoid gauging accuracy issues.

Two blending rules for predicting dielectric properties of simple mixtures were investigated and achieved excellent results when compared to direct measurements. These blending rules can help provide understanding into how particular jet fuel compositions will impact the FQIS performance. This can also provide insight into if additional empirical testing is needed to understand the dielectric vs. density relationship for a particular fuel composition.

This study clearly showed that different hydrocarbon classes have different dielectric permittivity and most importantly different slopes of dielectric vs. density relationship. This has further reinforced the need to move to a model in which the dielectric vs. density relationship is determined for each flight cycle to allow use of a wider range of fuel compositions and greater accuracy.

CRediT authorship contribution statement

Zhibin Yang: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **David C. Bell:** Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization. **Randall C. Boehm:** Writing – review & editing, Writing – original draft, Methodology. **Pedro Fischer Marques:** Writing – review & editing, Writing – original draft, Methodology. **Jessica A. Boze:** Writing – review & editing, Writing – original draft, Methodology. **Ilya V. Kosilkin:** Writing – review & editing, Writing – original draft, Methodology. **Joshua S. Heyne:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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16. Abstract

One of the challenges in developing 100% sustainable aviation fuels is the effect of synthetic blend components on the dielectric constant. Modern aircraft often employ capacitance-based gauging systems that rely on the dielectric constant of the fuel onboard to determine fuel quantity. Aircraft manufacturers have expressed concern over inaccuracies in fuel gauging attributable to variances in the dielectric constant between conventional jet fuels and 100% paraffinic sustainable aviation fuel. In our study, dielectric constant and density data were gathered from 172 conventional jet fuel samples to establish a baseline "experience range." Subsequently, thirty-five individual hydrocarbon molecules from the jet fuel range and nine fuels were acquired, characterized, and reported herein according to the Clausius-Mossotti relationship. Our findings indicate that different hydrocarbon group types exert varying effects on the Clausius-Mossotti relationship. To align with the established experience range for both the dielectric constant and the Clausius-Mossotti relationship, it appears that 100% drop-in SAF will need to incorporate some aromatic compounds. Finally, we explored two blending rules for the dielectric constant of jet fuel range hydrocarbons and achieved excellent coefficients of determination (R^2 values of 0.9942 and 0.9983, respectively).

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