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Preferential Vaporization Impacts on Lean Blow-Out of Liquid Fueled Combustors

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16. Abstract

Recent experimental works have shown that the global equivalence ratio defining lean blowout (LBO) in model gas turbine combustors correlates with the derived cetane number (DCN) of the tested fuel, which represents the chemical reactivity potential of the fuel, but additional physical and kinetic parameters of the fuel also have influence. The current work explores the significance of preferential vaporization impacts on LBO behaviors; i.e., rather than parameterizing the fuel by overall averaged fuel properties, it looks at DCN correlations based upon distillation properties prior to full vaporization. Preferential vaporization potentials of six fuels are evaluated by measuring the DCN values of five distillation cuts (each of 20% liquid distillation volume recovered). In spite of relatively large disparities in total fuel DCN values (~9.1), two petroleum-derived jet fuels are found to have nearly the same LBO equivalences, which is attributed to the relatively indiscernible difference of DCN values (~ 2) for the initial 20% distillation cut of each fuel. Trade-off impacts between fuel chemical and physical properties are demonstrated by comparing n-dodecane and Gevo-ATJ, which do not have preferential vaporization potential. LBO results suggest that fuel physical properties (particularly fuel boiling characteristics) predominantly control LBO behaviors at low air inlet temperature conditions, whereas fuel chemical properties appear to gain significance with increasing air inlet temperature. Further evidence of preferential vaporization effects on LBO is discussed with two surrogate mixtures formulated to emulate the fully pre-vaporized combustion behaviors of Jet-A, but having drastically different preferential vaporization potentials. Finally, the relationship between DCNs and LBO equivalence ratios is re-examined using the DCN values of initial 20% distillation cuts of all six fuels. The results display a significantly improved correlation, suggesting that the relevance of preferential vaporization on LBO can be significant for fuels that exhibit significant departure of the DCN for high volatile fractions (i.e., the initially vaporized constituents) in comparison to the overall fuel DCN.

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Abstract

Recent experimental works have shown that the global equivalence ratio defining lean blow-out (LBO) in model gas turbine combustors correlates with the derived cetane number (DCN) of the tested fuel, which represents the chemical reactivity potential of the fuel, but additional physical and kinetic parameters of the fuel also have influence. The current work explores the significance of preferential vaporization impacts on LBO behaviors; i.e., rather than parameterizing the fuel by overall averaged fuel properties, it looks at DCN correlations based upon distillation properties prior to full vaporization. Preferential vaporization potentials of six fuels are evaluated by measuring the DCN values of five distillation cuts (each of 20% liquid distillation volume recovered). In spite of relatively large disparities in total fuel DCN values (~ 9.1), two petroleum-derived jet fuels are found to have nearly the same LBO equivalences, which is attributed to the relatively indiscernible difference of DCN values (~ 2) for the initial 20% distillation cut of each fuel. Trade-off impacts between fuel chemical and physical properties are demonstrated by comparing n-dodecane and Gevo-ATJ, which do not have preferential vaporization potential. LBO results suggest that fuel physical properties (particularly fuel boiling characteristics) predominantly control LBO behaviors at low air inlet temperature conditions, whereas fuel chemical properties appear to gain significance with increasing air inlet temperature. Further evidence of preferential vaporization effects on LBO is discussed with two surrogate mixtures formulated to emulate the fully pre-vaporized combustion behaviors of Jet-A, but having drastically different preferential vaporization potentials. Finally, the relationship between DCNs and LBO equivalence ratios is re-examined using the DCN values of initial 20% distillation cuts of all six fuels. The results display a significantly improved correlation, suggesting that the relevance of preferential vaporization on LBO can be significant for fuels that exhibit significant departure of the DCN for high volatile fractions (i.e., the initially vaporized constituents) in comparison to the overall fuel DCN.

1. Introduction

Operating aviation gas turbine engines using liquid jet fuels intrinsically involves complicated multi-phase combustion behaviors associated with complex chemical kinetic characteristics coupled with spray injection, atomization/vaporization, turbulent mixing, and heat transfer phenomena [1-5]. Engine operating envelopes are typically delineated by near-limit combustion behaviors (e.g. flashback, lean blow-out, and high altitude relight) that are known to be strongly influenced by fuel properties [1-8]. The complex impacts of fuel properties are generally reflected in determining fuel certification standards [1] that specify nominal ranges for a significant number of fuel property indicators for aviation turbine fuels (rigorously evaluated through ASTM standard test specification [9, 10]). The specified indicators generally do not constrain the specific chemical species composing the fuel with the exception of a limited number of chemical class species that strongly contribute to sooting propensity.

The historical industry approach has typically categorized the properties relevant to near-limit combustion behaviors rather simply as either physical or chemical properties. The physical properties typically involve density, viscosity, surface tension (known to affect the spray atomization) and boiling characteristics (distillation parameters, known to affect liquid/vapor transformation rates). For fuel chemical properties, the current ASTM standard specification only evaluates three property indicators (hydrogen content, heat of combustion, and smoke point), which have recently been shown to be ineffective in characterizing fuel chemical kinetic characteristics [11]. Beyond these characterizations, little consideration has been given to how physical/chemical parameters might combine to affect local chemical kinetic reactivities other than through determining local fuel vapor/oxidizer equivalence ratios.

Understanding the relative significance of fuel chemical and physical properties on lean blow-out (LBO) has been of intense interest [6-8, 12-17]. Lefebvre (1985) [13] concluded that fuel physical properties were relatively more significant, based on extensive experimental tests using three petroleum-derived jet fuels (JP-4, JP-8, and No. 2 Diesel) and the commercially available atomizer/combustor concepts of the time. The underlying rationale for this conclusion was that fuel physical properties govern atomization quality and vaporization rates, whereas fuel chemical properties play only a minor role through slight variations in fuel heating values. However, recent experimental observations of LBO with petroleum-derived jet fuels, emerging alternative jet fuels, and their blends suggest that under a range of conditions chemical property effects may also be significant [7, 14-17]. This importance emerged as a strong correlation of LBO with the fuel derived cetane number (DCN), a parameter identified in earlier work as an indicator of chemical reactivity potential [11, 18-22].

This contradiction between the past and present measurements can be partly explained by improvements in atomization technologies in modern designs as well as increasing variabilities of properties for the fuels investigated more recently. **Figure 1** compares values of DCN and viscosity at -20 ^{o}C of both petroleum-derived and alternative jet fuels [11] as representative fuel chemical and physical properties, respectively, along with the variabilities of Jet-A, JP-8, and JP-5 reported in [23]. The chemical reactivity potential of alternative jet fuels as represented by their DCN values are found to vary substantially from the envelope of in-use petroleum-derived jet fuels, whereas their viscosity values are comparable to those of petroleum-derived fuels. **Figure 1** therefore suggests that the strong correlation between LBO and fuel physical properties, observed in [13], originates from testing only petroleum-derived fuels. All of the fuels tested in [13] display only a narrow variability in fuel chemical properties, but widely differing physical properties, spanning those for JP-4 and Diesel No. 2. On the other hand, the recent experimental studies on LBO for both petroleum-derived and alternative jet fuels considered a significantly larger variation in chemical properties, as shown in **Fig. 1.**

As noted above, the historical approach to considering impacts of fuel chemical and physical properties on LBO *separately* in a relative/correlative manner has been widely employed [6, 7, 12-17]. However, this approach often fails to fully elucidate the observed LBO behaviors. Considering that the initial droplet diameter of 20 – 50 μm typical of most fuel atomization methods [24], the characteristic time scale for evaporation (τ_{evap}) can be approximated as 1 – 10 milliseconds [25-27] at ~700 K (also highly sensitive to the pressure condition), which is comparable to the characteristic flow time scale (τ_{flo}) between the fuel atomizer exit plane and the leading edge of the flame front in most of gas turbine combustors. When $\tau_{evap} > \tau_{flo}$, it is expected that the fuel droplets formed might not fully pre-vaporize, resulting in the presence of droplets within the flame region. Moreover, the vaporization characteristics at the droplet surface over their time history may result in so-called "preferential vaporization", wherein the lighter more volatile fuel components leave the liquid surface more rapidly than the droplet heavier components, i.e., the local vaporized fractions do not align with the initial liquid phase fractions, and heavier components disproportionately remain in the liquid phase. The relevant questions to consider are how the preferential vaporization of the lighter components, both in terms of their ability to create locally flammable conditions and their chemical reactivity potential, compared to that of the original fuel and/or how the heavy end affects LBO characteristics.

Although the potential impact of preferential vaporization on LBO behaviors described above appears possible conceptually, its relevance has not been well characterized previously, primarily due to the technical challenges in formulating meaningful experiments and fuel blends. Numerical investigations using relatively simplified configurations have indicated an importance (e.g. [28]), but a fundamental understanding (supported by experimental evidence) of coupling impacts between fuel chemical and physical properties for real fuels remains a challenge. In this regard, the surrogate approach provides opportunities to evaluate the potential preferential vaporization impacts on LBO behaviors by permitting control over chemical potential reactivity while varying fuel physical properties. Extensive studies [18-20, 22] have shown that the pre-vaporized combustion behaviors of fuel/air mixtures can be successfully emulated by a surrogate formulated by matching the combustion property targets (CPT's) of DCN, H/C (molar) ratio, average fuel molecular weight (MW), and smoke point (SP). In previous work using CPT concepts, [22], we showed that two surrogate mixtures exhibiting identical pre-vaporized combustion behaviors as a jet fuel target, but that have drastically different preferential vaporization characteristics, can be formulated by selecting different surrogate components.

The primary goal of this paper is to evaluate the impact(s) of preferential vaporization on LBO behaviors through the characterization of preferential vaporization potential combined with surrogate fuel formulation methods based upon the CPT approach. Our recent study [15] summarized the first-order relative significance of fuel chemical and physical properties on LBO behaviors as a function of air inlet temperature by examining a total of eighteen different fuels, spanning a wide range of chemical and physical properties. The current work focuses on only six of the fuels in terms of their LBO behaviors and performs additional analyses based upon their distillation properties to evaluate preferential vaporization impacts. The LBO characteristics regarding preferential vaporization potential are analyzed for 1) two petroleum-derived jet fuels (Jet-A and JP-5), 2) two chemically well-defined fuels (n-dodecane and an alternative renewable fuel, Gevo-ATJ [29, 30], which is essentially a mixture of iso-dodecane and iso-cetane), and 3) two surrogate component mixtures, previously formulated to emulate the fully pre-vaporized combustion behaviors of Jet-A [22]. The prior LBO results are considered in light of new experimental results that characterize the chemical reactivity potential (DCN) for fractional cuts of each fuel over their respective distillation curves.

2. Experiment and Methodology

A total of six fuel samples were prepared by the US Air Force Research Laboratory (AFRL) and shipped to Georgia Tech (GIT) and University of South Carolina (USC) to perform the LBO measurements and fuel property characterizations, respectively. As discussed above and shown in [23], fuel properties vary considerably, even for petroleum-derived jet fuels having different fit-for-purpose applications (e.g. Jet-A, JP-5, etc.). To avoid confusion, AFRL has established a fuel property database by assigning a POSF number of each fuel received and subsequently analyzed. The term "POSF" originates from an earlier name of the AFRL Fuels Branch's organizational designation [31]. The specific fuels used in this study are Jet-A POSF 10325, JP-5 POSF 10289, Gevo-ATJ POSF 10151 (POSF 11498 is identical in terms of indicators to POSF 10151), n-dodecane, Surrogates 1 and 2, formulated by combustion property target (CPT) methodology as described in [22] to share the same CPT's as Jet-A POSF 10325. The surrogate mixtures were prepared at AFRL based on the mixture specifications provided by USC.

2.1. Lean blow-out (LBO) experiment

LBO measurements for each fuel were measured in the combustion test rig at GIT. The GIT facility includes a pre-conditioned air supply, fuel supply, an optically accessible pressure vessel and liner, an interchangeable fuel injector, and an exhaust section. Details of the GIT facility are reported elsewhere [15-17], thus only a brief description is provided here. **Figure 2** shows the schematic of GIT test rig, which was designed specifically to mimic aircraft gas turbine engines as a model combustor.

The air supply and preconditioning system control the air inlet temperature within ±10 K through use of an electric heater and heat exchanger. The air temperature is continuously monitored at 35 cm upstream of the bulkhead (fuel injector head) location of the combustor section. Primary air is introduced directly to the combustor (30.5 cm long and 105 inner diameter quartz) section through an annular swirler upstream of the atomizer to promote spray atomization and vaporization. After passing through a heat exchanger to maintain temperature at 320 K, secondary air is introduced to the liner surrounding the quartz combustor section for the cooling of the pressure vessel and optical windows. The hot combustion products are merged with the secondary air at the end of the combustion liner. The exhaust gases finally exit the combustor through a choked orifice plug which maintain the system pressure at 345 kPa. Air mass flow rates are measured by Rosemount vortex flowmeters.

Three air inlet temperatures (300, 450, and 550 K) were used to vary the extent of fuel spray vaporization achieved for each fuel. At the inlet of the combustor, a stainless-steel nozzle assembly (bulkhead) similar to the one used in [32], is located to inject liquid fuel through a pressure-type atomizer (McMaster-Carr, product number 3178K45), having an orifice diameter of 0.51 mm. Since the stainless-steel nozzle assembly is not actively cooled during the experiments, four thermocouples are mounted at the surface of nozzle assembly to monitor the temperature (bulkhead temperature). Estimated uncertainties in overall measured fuel/air ratio are 3%.

It is understood that heat transfer from the combustor hardware can influence the equivalence ratio at which the flame blows out [15-17, 33]. Therefore, the experimental procedure was designed to parametrize these heat transfer effects by using the bulkhead temperature to characterize the combustor thermal state. This process involved first raising the bulkhead temperature by burning a steady-state stable flame. Then the fuel flow rate was gradually decreased until LBO occurred. Following a blowout occurrence, the flame was re-ignited and LBO measurements continued to be acquired. The reduced flame temperatures of the weakly burning near-blowout flames, compared to the initial stable flame, caused the bulkhead temperature to decrease over time. Eventually, the heat gained by the combustor hardware from the stable flame was lost and the bulkhead temperature converged to an equilibrium value. In order to gather LBO measurements at cold combustor conditions, the fuel flow was temporarily terminated, thereby allowing the bulkhead temperature to drop well below its equilibrium value. The flame was then reignited and the blowout-reignition process resumed while the remainder of the LBO measurement were taken. Consequently, the equivalence ratio at LBO was obtained at various bulkhead temperatures for a single fuel, and this procedure was then repeated for each of the remaining fuels. Approximately twenty LBO measurements per fuel were gathered on each day that the experiment was repeated. Further details of the experimental procedure can be found in [15-17].

The air velocity at the exit of the nozzle (combustor inlet) is estimated as ~ 60 m/s based on air mass flow rates and combustor geometry. LBO measurements were obtained consistently for all fuels tested by regulating fuel mass flow rates while maintaining air mass flow rate constant, enabling the following analyses on LBO behaviors regarding preferential vaporization potential of fuels.

2.2. Characterization of Preferential Vaporization Potential

The preferential vaporization potentials of fuels have been evaluated at USC by preparing distillation cuts through an ASTM D86 distillation device [34] and measuring the derived cetane number (DCN) of the fuel and each distillation cut through the ASTM D6980 standard [35].

The ASTM D86 distillation method requires heating a glass container (~ 250 mL) of liquid fuel with an electric heater, while determining the vaporization temperature at the top exit of the container. The vapor is then introduced to a heat exchanger tubing, which is located in the chilled water bath. In order to ensure complete condensation of the vaporized sample at the collection glass container, the flow is cooled with a chilled (273 K) water flow maintained by a circulating bath (Cole-Parmer, Polystat UX-12122-62). Five distillation cuts of ~20 % volume each of the original fuel sample are obtained along with their beginning and ending vapor temperatures.

Figure 3 compares the measured distillation characteristics of Jet-A POSF 10325 to those reported by US Air Force Research Laboratory (AFRL) [7]. Considering that the current ASTM D86 methodology has inevitable uncertainty associated with its configuration and the use of liquid volume as a parameter as discussed in [36-38], the results have a maximum deviation of 9 K, which is sufficiently accurate for the present work. During the distillation measurement, the individual five distillation cuts are collected along the distillation curve by replacing the receiving container in every 20% liquid volume recovered point, as seen in the inset of **Fig. 3**. Interestingly, the initial four distillation cuts of the Jet-A were essentially colorless, whereas the last bin sample exhibited a brownish yellow color (perhaps due to sulfur-containing species or fuel additives). Although not shown in the figure, the distillation characteristics of two other real fuels (JP-5 POSF 10289 and Gevo-ATJ) have been similarly produced and the distillation curve data compared to the results reported by AFRL.

The chemical reactivity potential of the actual fuels, as well as each of their distillation cuts, were characterized by DCN measurements performed using an ignition quality tester (IQT). The

DCN is a global/relative measure of the autoignition propensity of a fuel determined by an IQT, which records ignition delay time associated with the injection of a liquid fuel sample (a constant volume) into a heated (~ 830 K) constant volume chamber containing pressurized air at ~ 22 atm. Though cetane number variants such as DCN have been historically developed for diesel applications, we have extensively utilized the DCN to compare the chemical kinetic reactivity potential of single fuel components, components mixtures, petroleum-derived jet fuels, alternative jet fuels, and their mixtures. The DCN has been used one of the Combustion Property Targets (CPT's) in surrogate mixture formulation [18-20, 39] to emulate fully pre-vaporized combustion behaviors of real fuels. The DCN has a direct correlation with low-temperature reactivity due to the thermodynamic condition employed in the IQT [11], but we have also shown that the value reflects high-temperature reactivity as well, due to the strong sensitivity of DCN to $(CH_2)_n$ functional group presence in the fuel as shown in [22]. A large fraction of $(CH_2)_n$ functional groups indicates the presence of large fractions of normal-alkanes that rapidly produce a large reactive radical pool at high temperatures through oxidative pyrolysis [11, 22]. Although the relevance of low-temperature reactivity to the gas turbine application is still in debate, there is strong evidence that intermediate temperature chemistry occurring above ~750 K also affects radical pool development at higher pressures. Here, we utilize the DCN values of both the whole fuel sample and their distillation cuts as a chemical reactivity potential indicator.

3. Results and Discussion

In the following, we present and discuss comparative results for three sets of two fuels and their implications regarding the significance of preferential vaporization on the LBO observations. Through their comparative properties in terms of distillation curve, and DCN's for each distillation fraction and whole fuel, each set of fuels emphasize different aspects with regard to the impact of physical and chemical properties on the observed LBO behaviors. First, we contrast the LBO behaviors of two petroleum-derived jet fuels (Jet-A POSF 10325 and JP-5 POSF 10289). We then contrast the results obtained for two fuels that have little or no variation in DCN as a function of distillation. The two fuels used for this case are technical grade n-dodecane, and a renewable fuel, Gevo-ATJ. Then, we compare the results obtained for two surrogate fuel compositions, each which closely emulates Jet-A POSF 10325 in terms of their overall fuel DCN, but have very different distributions of DCN over their distillation fractions.

Finally, correlations between the LBO boundaries of all six fuels and both the whole fuel DCN and the DCN of the first 20 % distillation cut are compared and discussed.

3.1. LBO behaviors of two petroleum-derived jet fuels

Figure 4 displays the raw data for the LBO equivalence ratios for (a) Jet-A POSF 10325, (b) JP-5 POSF 10289, (c) n-dodecane, (c) Gevo-ATJ POSF 10151 as functions of measured bulkhead temperature at three different air inlet temperatures. In general, at each air inlet temperature, the determined LBO equivalence ratios decrease slightly with increasing scatter as bulkhead temperature increases. This trend can be clearly seen for n-dodecane and Gevo-ATJ, as well as two surrogate mixtures (see supplementary material), whereas two petroleum-derived jet fuels exhibit relatively large scattering in the relationship between LBO equivalence ratios and bulkhead temperatures.

The relationship between the measured LBO equivalence ratio and the bulkhead temperature has been extensively discussed previously [15-17]. It was hypothesized that the observed dependence on bulk head temperature resulted from radiative thermal feedback from flame regions to the fuel atomizer, raising the sensible enthalpy of the atomizing fuel and decreasing fuel viscosity (smaller mean droplet size at higher initial temperatures). In the case of the two petroleum-derived fuels, the larger scattering in LBO values at higher bulk head temperature conditions could be attributed to the thermal stability of specific chemical components in the fuel sample and/or the excessive heating of liquid fuel inside the injector beyond fuel boiling temperature, which would induce significant changes in spray dynamics. Although the change of spray dynamics due to the thermal stability of fuel and the consequent impacts on flame stability could be an interesting research subject, we haven't pursued this route further, since it is beyond the scope of this study.

For the sake of simplicity and avoiding further consideration of the source(s) for the scatter, the average values of the measured LBO equivalence ratios over the following bulkhead temperature ranges ( ) are utilized in subsequent analyses;

- For $_{air}$ = 300 K, 450 K < < 550 K
- For $_{air}$ = 450 K, 500 K < < 650 K
- For $_{air}$ = 550 K, 600 K < < 750 K

Considering that the LBO value for any particular fuel and air temperature is stochastic in nature (due to the complex nature of multi-phase turbulent combustion), the scatter in data are treated as a random uncertainty. Bias errors resulting from the chosen specified temperature ranges for noted were carefully considered. Although the absolute average values of LBO equivalence ratios are dependent on the specified bulkhead temperature ranges, generic trends for the following analyses remained unchanged, enabling the qualitative assessment. Similar analyses with narrower bulk head temperature ranges (Δ = 50 K) are included in the supplementary material that also qualitatively demonstrate the same behaviors to those using the temperature ranges specified above.

Table 1 summarizes the whole real fuel DCN and pertinent physical property data for Jet-A POSF 10325 and JP-5 POSF 10289. The difference in DCN values between Jet-A POSF 10325 and JP-5 POSF 10289 imply significantly greater chemical reactivity for fully pre-vaporized Jet-A POSF 10325 in comparison to JP-5 POSF 10289. The higher H/C ratio of Jet-A POSF 10325 is consistent with the lower value of TSI (indicative of less aromatic contents) compared to JP-5 POSF 10289. The data comparisons suggest that the LBO equivalence ratio for Jet-A POSF 10325 might be lower than that for JP-5 POSF 10325, based the recent correlation of real jet fuel LBO equivalence ratio and DCN [7, 15-17]. On the other hand, the fuel physical property comparisons also suggest that the LBO equivalence ratio of Jet-A POSF 10325 should be lower than for JP-5 POSF 10289, based on the work by Lefebvre [13] and the lower density and lower boiling temperatures compared to JP-5 POSF 10289. **Figure 5** compares the measured LBO equivalence ratios of the two petroleum-derived fuels as a function of air inlet temperature, along with their standard deviations, maximum and minimum values within the specified bulkhead temperature ranges. In deference to the above hypotheses, the summarized results show essentially no discernible differences in the averaged LBO data for the two fuels.

However, the results are entirely consistent with the consideration that preferential effects control the relative LBO behaviors. **Figure 6** compares the measured DCN values of each of the five distillation cuts for Jet-A POSF 10325 and JP-5 POSF 10289, along with the DCN values of each whole fuel sample (dashed lines). The data demonstrate that for each fuel, the fuel reactivity potential (DCN) increases substantially from light- to heavy-end distillation cuts defining over the distillation curve. Although the DCN values of whole sample for Jet-A POSF 10325 and JP-5 POSF 10289 are found to differ by ~ 9 DCN units, the measured DCN values of the initial light-end distillation cuts are within ~ 2 DCN units. Under conditions where preferential vaporization dominates the determination of the LBO equivalence ratio, one would expect similar LBO equivalence ratios for the two fuels given that all other physical properties were the same.

The potential impacts of fuel physical properties (e.g. density, viscosity, surface tension, distillation curve) on atomization and vaporization rate cannot be isolated from chemical variations in the vaporized fractions in the current comparison, as the two petroleum-derive fuels are also different in the physical properties themselves [7, 15-17]. However, recent non-combustion experimental measurements at similar fuel atomization temperatures and atmospheric pressure have shown that these two fuels exhibit similar spray properties, such as mean droplet diameter and velocity [24].

As discussed earlier, however, the operating global equivalence ratio at each air inlet temperature is gradually reduced until LBO is achieved, resulting in a decreasing bulk flame temperature and radiating volume. Consequently, it is likely that heat transfer from the flame volume to the atomization region also decreases, potentially resulting in lower fuel atomization temperature, higher fuel atomization viscosity, larger mean droplet size, and slower initial droplet vaporization rates. It is possible that atomized droplet lifetimes are larger and flame stabilization becomes affected more significantly by the chemical properties of the initial light-end fuel fraction.

While the significance of preferential vaporization on observed LBO behaviors can be speculated from the comparison of data for these two petroleum-derived jet fuels, the significance of chemical fuel properties related to preferential vaporization remains unclear. In this regard, the comparison of data for two well-defined fuels, n-dodecane and Gevo-ATJ, provide an opportunity to evaluate the sole impact of fuel chemical property on LBO, since both fuels have essentially no DCN differences over their vaporization history and almost identical fuel physical properties other than boiling temperatures of their components.

3.2. LBO behaviors of n-dodecane and Gevo-ATJ

Gevo-ATJ is composed of only two iso-alkane components, iso-dodecane (> 85% in liquid volume) and iso-cetane [29, 30], each having almost identical DCN's. Therefore, there is essentially no variation in DCN from that of the overall fuel over the distillation curve. The fully pre-vaporized chemical kinetic behaviors of iso-dodecane and iso-cetane are also very similar in terms of premixed laminar adiabatic flame temperatures, laminar diffusion flame extinction limits, and homogeneous reflected shock ignition delay times [29]. Consequently, it is expected that Gevo-ATJ has negligible potential effects through preferential vaporization as far as only chemical kinetic reactivity is concerned.

Table 2 summarizes key fuel properties of n-dodecane and Gevo-ATJ, emphasizing the nearly identical fuel physical properties but vastly different DCNs. Therefore, the LBO behavior comparisons between n-dodecane and Gevo-ATJ weights the significance of fuel chemical reactivity potential (DCN) and physical properties as a function of fuel and air inlet temperature without any impacts from preferential vaporization. **Figure 7** summarizes the data and clearly shows that the measured equivalence ratios at LBO for n-dodecane are always lower than those for Gevo-ATJ. At an air inlet temperature of 300 K, the measured equivalence ratios at LBO for n-dodecane and Gevo-ATJ are 0.39 and 0.41, respectively (within ~ 0.02 of one another). With increasing the air inlet temperature, the difference becomes greater, (0.024 at 450 K and 0.027 at 550 K), as clearly shown in normalized equivalence ratio. At 550 K of air inlet temperature, the percentage difference of LBO equivalence ratios reaches ~ 10 %, which is indeed comparable to the typical differences (~ 10 – 20 %) of laminar flame speeds [40, 41] and flame extinction limits [42, 43] between n-alkanes and iso-alkanes.

The relative impact of fuel chemical properties versus physical properties on LBO behaviors has been demonstrated and discussed previously based upon a database for a much larger number of fuels [15]. At lower air inlet temperature, the relatively slower fuel vaporization rates render LBO behaviors increasingly sensitive to fuel physical properties, as atomization and vaporization become the rate limiting processes. Only when these processes are fast relative to kinetics, will kinetic processes be limiting, as in the case of perfectly premixed systems. Consequently, with increasing air temperature, LBO behaviors become increasingly correlated to fuel chemical reactivity potential (DCN), as the stabilizing flame criteria shifts from non-premixed to partially premixed combustion characteristics. These arguments support the larger percent differences in the LBO equivalence ratios of n-dodecane and Gevo-ATJ with increasing air temperature conditions.

3.3. Comparison between target jet fuel and its surrogate mixtures

Additional insights can be obtained by comparing the LBO equivalence ratios for two surrogate fuel mixture that have been formulated previously in [22] to emulate the fully pre-vaporized combustion behaviors of Jet-A POSF 10325. The mixtures were derived using CPT formulation methodologies described in [18, 19]. The properties of the two surrogate mixtures are summarized in **Table 3**.

Surrogate 1 is composed of n-dodecane, iso-octane, and 1,3,5-trimethylbenzene, whereas surrogate 2 was purposely formulated to amplify potential preferential vaporization differences of the two fuels by replacing n-dodecane with n-hexadecane as the n-alkane component. Both predictions using a chemical functional group descriptor developed previously [22, 44] and recent experimental results in well-stirred reactor experiments [45] suggest that the global combustion behaviors of fully pre-vaporized fuel/air mixtures of Jet-A POSF 10325 can be successfully emulated by these two surrogates.

The DCN values for the five distillation cuts (20% recovered each) for Jet-A POSF 10325 and two surrogate mixtures are compared in **Fig. 8**. Distillation curves and chemical composition variations of the two surrogate mixtures are calculated by employing the partial equilibrium assumption between vapor and liquid phase compositions as a function of temperature, as described in [22]. Then, DCN value of each distillation cut is estimated with the known chemical composition by using the regression model based on chemical functional group descriptor previously developed in [22]. The DCN value can be predicted within an uncertainty of 3.5 units, defined as standard deviation between the measured and predicted values in the regression analysis. Although the DCN values of each whole fuel have been developed to be the same, the comparison shows that the DCN value for the initial distillation cuts of two surrogates vary significantly, as a result of the surrogate component substitution described earlier. The initial 20 % distillation cut for surrogate 1 is estimated to be composed of 11% n-dodecane, 63% iso-octane, and 26% 1,3,5-trimethylbenzene, forecasting a mixture DCN of 28.7. The surrogate 2 initial distillation cut is estimated to be 1% n-hexadecane, 79% iso-octane, and 20% 1,3,5-trimethlybenzene, forecasting a DCN of 19.1.

Figure 9 compares the percent differences in LBO equivalence ratio data for the two surrogate mixtures with the measurements for Jet-A POSF 10325, as a function of air inlet temperature. The error bars in the figure are the standard deviation of multiple measurements divided by the average value of LBO measurements in the experimental plateau region (as described earlier). The comparison indicates that LBO is influenced by preferential vaporization more significantly at lower air inlet temperature. Although two surrogates have relatively lower boiling temperatures compared to Jet-A POSF 10325 (**Table 3**), both surrogates 1 and 2 show higher LBO equivalence ratios at 300 K and 450 K air inlet temperature conditions than those of Jet-A, while surrogate 2 exhibits an even higher LBO equivalence ratio over surrogate 1. However, at 550 K air inlet temperature, both surrogates result in essentially the same small deviation from the LBO equivalence ratio of Jet-A POSF 10325 target fuel.

Considering the results shown in both **Figs. 8 and 9**, a macroscopic comparison suggests that fuel chemical and physical properties couple through preferential vaporization effects on local fuel/oxidizer equivalence ratios as well as chemical reactivity at low air inlet temperatures, while the chemical properties of the entire fuel sample emerge as dominant factor at higher air inlet temperatures, where the vaporization of the fuel spray becomes closer to completion prior to the flame front region.

To further evaluate the impacts of preferential vaporization, the linear regression trend developed earlier of LBO equivalence ratios with whole fuel DCN (as reported in [7, 15-17]) is modified to compare the data for all six of the current fuels. **Figure 10a** shows the aforementioned comparison of the experimentally observed LBO equivalence ratios and measured DCN values for each of the six fuels. **Figure 10b** considers the same experimental LBO equivalence ratio data but plots it against the DCN values for the initial 20 % liquid volume distillation cuts of each of the six fuels.

The impacts of the chemical reactivity differences from preferential vaporization on LBO are clearly evident through comparison of the two figures. Firstly, the linear correlation coefficients associated with utilizing whole fuel DCNs are substantially improved upon by substitution of the DCN values of the initial 20 % liquid volume distillation cuts. Significant improvements in the linear correlation coefficients for the cases of 300 K and 450 K air inlet temperatures suggest that LBO behaviors are considerably affected by the preferential vaporization. Although a 550 K air inlet temperature is slightly higher than (or comparable to) end point distillation temperatures of all tested fuels, the improved correlation coefficients also suggest that preferential vaporization still affects LBO behaviors.

Secondly, the comparison shown in **Fig. 10b** indicates that the LBO equivalence ratios determined for Jet-A POSF 10325 are considerably affected by the preferential vaporization impact, whereas those for JP-5 POSF 10289 are relatively less influenced due to the relative differences in DCN values between whole fuel samples and their initial distillation cuts. Lastly, the significance of preferential vaporization impacts is clearly demonstrated by the data for the two surrogate mixtures (Surrogates 1 and 2) compared to the Jet-A POSF 10325 results.

The results shown here are significant in terms of addressing the fidelity of any CFD simulation with fuel-specific chemical kinetic models (either detailed or reduced/compacted) that *do not* permit emulating reactivity potential (DCN) variations over the fuel distillation curve. Currently, nearly all numerical modeling predictions employ chemical kinetic models that treat the fuel as a single molecular construct, C_nH_m, coupled with an empirical approach to emulate vaporization (distillation curve) properties. Particularly in cases where a large deviation of DCN over the distillation curve occurs in comparison to the value for the whole fuel itself, the above results show the limitations of the single fuel molecule approach, even if a prescribed distillation curve is artificially developed to embody the amount of vaporization as a function of droplet heating. This deficiency can be expected to be particularly important in cases where droplets are only partially pre-vaporized prior to burning, and so will vary with degree of fuel atomization and air temperature.

The analyses presented in this paper rely on a phenomenological interpretation based on correlations of macro-LBO behavior observed in a relatively large rig scale model combustor. Although the analyses strongly suggest the significance of preferential vaporization impacts on LBO behaviors, the use of a relative scale (DCN) for chemical reactivity of each fuel/distillation fraction limits any quantitative evaluation of preferential vaporization impacts. Considering that the correlation doesn’t indicate the causation, further fundamental investigations and detailed local flow/flame characterization will be definitely necessary to evaluate preferential vaporization impacts conclusively and quantitatively. Nonetheless, the analyses presented here provide strong support that preferential vaporization effects are important regarding LBO behaviors of fuels.

4. Conclusion

The significance of preferential vaporization on lean blow-out (LBO) behaviors has been investigated by evaluating the preferential vaporization potentials of six different fuels. Each fuel was distilled and the DCN values of five distillation cuts (20% liquid volume recovered, prepared by ASTM D86 approach) for two petroleum-derived jet fuels (Jet-A POSF 10325 and JP-5 POSF 10289) were determined using an ignition quality tester (IQT) and ASTM D6890 procedures.

The measured DCN values of the initial 20% distillation cuts for two jet fuels found to be similar (within ~2 DCN unit), in deference to the relatively large disparity of DCN values (~9.1 difference) of each whole fuel. This measured DCN similarity of initial distillation cuts among two petroleum-derived jet fuels gives support to the experimentally observed similarity of the equivalence ratios at LBO for the two fuels, but the actual significance remained inconclusive due to the differences in other physical properties.

Trade-off impacts between fuel chemical and physical properties were further examined by analyzing the behaviors of two fuels (n-dodecane (high DCN) and Gevo-ATJ (low DCN)) having similar physical properties and insignificant variations in chemical reactivity potential (DCN) over their distillation curves. The comparison of LBO behaviors suggests that fuel physical property impacts (particularly fuel boiling characteristics that contribute to local fuel/oxidizer equivalence ratio formation) dominate the LBO behaviors at low air inlet temperature condition, whereas fuel chemical reactivity potential differences begin to appear as a dominant factor affecting the LBO behavior at increasing air inlet temperatures (as more fully pre-vaporized conditions are approached).

Finally, two surrogate mixtures were tested that were formulated to emulate global combustion behaviors of fully pre-vaporized fuel/air mixtures of Jet-A POSF 10325. The surrogate mixtures shared the same whole fuel CPT’s, including DCN, of the real fuel, but had drastically different preferential vaporization characteristics. The measured equivalence ratios at LBO of the two surrogate mixtures compared to that of Jet-A POSF 10325 clearly shows that the surrogate mixtures could not emulate the LBO behaviors of Jet-A POSF 10325 due to pronounced preferential vaporization impacts at low air inlet temperatures. However, the agreement for each surrogate result with those for the real fuel is improved with increasing air inlet temperature alluding to a LBO controlling transition from fuel physical properties to chemical properties. Considering that the preferential vaporization impacts originate from a strong coupling of both fuel chemical and physical properties, the linear regression relationship of equivalence ratio at LBO with real fuel DCN was re-examined by substituting DCN values for the initial 20% distillation cuts of all fuels tested here. The substitution results in a significantly improved linear dependence of the data suggesting that the equivalence ratio at LBO is controlled not only by vaporization potential (lower initial distillation temperatures), but the chemical reactivity potential (DCN) of the initially vaporized materials.

Although the analyses presented in this paper are primarily based on the phenomenological interpretations on data collected for only six fuels, the implications of the results are significant to numerical modeling aspects for multi-phase combustion predictions that involve real fuels. The present results suggest that both chemical kinetic model constructs and spray sub-models in CFD simulations need to be more fully considered in order to properly account for the preferential vaporization impacts on local fuel/oxidizer mixture formation as well as on local chemical reactivity properties. Finally, the present study also suggests that the surrogate approach can be utilized to evaluate the relative significance(s) of fuel chemical and physical properties on combustor performance experimentally, in a manner not presently possible through numerical modeling approaches applied to multi-phase combustion systems.

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References

[1] F.L. Dryer, Chemical kinetic and combustion characteristics of transportation fuels, Proceedings of the Combustion Institute 35 (2015) 117-144.

[2] M. Stöhr, I. Boxx, C. Carter, W. Meier, Dynamics of lean blowout of a swirl-stabilized flame in a gas turbine model combustor, Proceedings of the Combustion Institute 33 (2011) 2953-2960.

[3] A. Ateshkadi, V.G. McDonell, G.S. Samuelsen, Lean blowout model for a spray-fired swirl-stabilized combustor, Proceedings of the Combustion Institute 28 (2000) 1281-1288.

[4] S.J. Shanbhogue, S. Husain, T. Lieuwen, Lean blowoff of bluff body stabilized flames: Scaling and dynamics, Progr. Energy Combust. Sci. 35 (2009) 98-120.

[5] T.C. Lieuwen, Unsteady combustor physics, Cambridge University Press2012.

[6] W.-W. Kim, J.J. Lienau, P.R. Van Slooten, M.B. Colket, R.E. Malecki, S. Syed, Towards Modeling Lean Blow Out in Gas Turbine Flameholder Applications, Journal of Engineering for Gas Turbines and Power 128 (2004) 40-48.

[7] M.B. Colket, J. Heyne, M. Rumizen, M. Gupta, A. Jardines, J.T. Edwards, W.M. Roquemore, G. Andac, R. Boehm, J. Zelina, J. Lovett, J. Condevaux, S. Bornstein, N. Rizk, D. Turner, C. Graves, M.S. Anand, R. Williams, Fang Xu, J.M. Tishkoff, C. Li, J.P. Moder, R. Anthenien, D. Friend, P. Chu, R. Kamin, Z. Haq, P. Serino, M. Domen, C.-B.M. Kweon, V. Sankaran, J. Cohen, W. Chishty, P. Canteenwalla, A. Corber, An Overview of the National Jet Fuels Combustion Program, 54th AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics 2016.

[8] L. Esclapez, P.C. Ma, E. Mayhew, R. Xu, S. Stouffer, T. Lee, H. Wang, M. Ihme, Fuel effects on lean blow-out in a realistic gas turbine combustor, Combust. Flame 181 (2017) 82-99.

[9] ASTM D7566, Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons, ASTM International, 2013.

[10] ASTM D1655-18a, Standard Specification for Aviation Turbine Fuels, ASTM International, 2018.

[11] S.H. Won, P.S. Veloo, S. Dooley, J. Santner, F.M. Haas, Y. Ju, F.L. Dryer, Predicting the global combustion behaviors of petroleum-derived and alternative jet fuels by simple fuel property measurements, Fuel 168 (2016) 34-46.

[12] A.H. Lefebvre, Fuel effects on gas turbine combustion - Liner temperature, pattern factor and pollutant emissions, 20th Joint Propulsion Conference, American Institute of Aeronautics and Astronautics1984.

[13] A.H. Lefebvre, Fuel Effects on Gas Turbine Combustion—Ignition, Stability, and Combustion Efficiency, Journal of Engineering for Gas Turbines and Power 107 (1985) 24-37.

[14] S. Stouffer, T. Hendershott, J.R. Monfort, J. Diemer, E. Corporan, P. Wrzesinski, A.W. Caswell, Lean Blowout and Ignition Characteristics of Conventional and Surrogate Fuels Measured in a Swirl Stabilized Combustor, 55th AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics2017.

[15] N. Rock, I. Chterev, B. Emerson, S.H. Won, J. Seitzman, T. Lieuwen, Liquid Fuel Property Effects on Lean Blowout in an Aircraft Relevant Combustor, Journal of Engineering for Gas Turbines and Power 141 (2019) 071005-071005-071013.

[16] N. Rock, I. Chterev, B. Emerson, J. Seitzman, T. Lieuwen, Blowout Sensitivities in a Liquid Fueled Combustor: Fuel Composition and Preheat Temperature Effects, ASME Turbo Expo 2016: Turbomachinery Technical Conference and Exposition, Seoul, South Korea, 2016, pp. V04AT04A022.

[17] N. Rock, I. Chterev, T. Smith, H. Ek, B. Emerson, D. Noble, J. Seitzman, T. Lieuwen, Reacting Pressurized Spray Combustor Dynamics: Part 1 — Fuel Sensitivities and Blowoff Characterization, ASME Turbo Expo 2016: Turbomachinery Technical Conference and Exposition, Seoul, South Korea, 2016, pp. V04AT04A021.

[18] S. Dooley, S.H. Won, M. Chaos, J. Heyne, Y. Ju, F.L. Dryer, K. Kumar, C.-J. Sung, H. Wang, M.A. Oehlschlaeger, R.J. Santoro, T.A. Litzinger, A jet fuel surrogate formulated by real fuel properties, Combust. Flame 157 (2010) 2333-2339.

[19] S. Dooley, S.H. Won, J. Heyne, T.I. Farouk, Y. Ju, F.L. Dryer, K. Kumar, X. Hui, C.-J. Sung, H. Wang, M.A. Oehlschlaeger, V. Iyer, S. Iyer, T.A. Litzinger, R.J. Santoro, T. Malewicki, K. Brezinsky, The experimental evaluation of a methodology for surrogate fuel formulation to emulate gas phase combustion kinetic phenomena, Combust. Flame 159 (2012) 1444-1466.

[20] S. Dooley, S.H. Won, S. Jahangirian, Y. Ju, F.L. Dryer, H. Wang, M.A. Oehlschlaeger, The combustion kinetics of a synthetic paraffinic jet aviation fuel and a fundamentally formulated, experimentally validated surrogate fuel, Combust. Flame 159 (2012) 3014-3020.

[21] S.H. Won, S. Dooley, P.S. Veloo, H. Wang, M.A. Oehlschlaeger, F.L. Dryer, Y. Ju, The combustion properties of 2,6,10-trimethyl dodecane and a chemical functional group analysis, Combust. Flame 161 (2014) 826-834.

[22] S.H. Won, F.M. Haas, S. Dooley, T. Edwards, F.L. Dryer, Reconstruction of chemical structure of real fuel by surrogate formulation based upon combustion property targets, Combust. Flame 183 (2017) 39-49.

[23] Petroleum Quality Information System (PQIS) 2013 Annual Report, Defense Logistics Agency Energy, Ft. Belvoir, VA, 2013.

[24] A. Bokhart, D. Shin, N.S. Rodrigues, P. Sojka, J.P. Gore, R.P. Lucht, Spray Characteristics of a Hybrid Airblast Pressure-Swirl Atomizer at Near Lean Blowout Conditions using Phase Doppler Anemometry, 2018 AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics2018.

[25] C.K. Law, Recent advances in droplet vaporization and combustion, Progr. Energy Combust. Sci. 8 (1982) 171-201.

[26] J. Tamim, W.L.H. Hallett, A continuous thermodynamics model for multicomponent droplet vaporization, Chem. Eng. Sci. 50 (1995) 2933-2942.

[27] S.S. Sazhin, Modelling of fuel droplet heating and evaporation: Recent results and unsolved problems, Fuel 196 (2017) 69-101.

[28] A. Stagni, L. Esclapez, P. Govindaraju, A. Cuoci, T. Faravelli, M. Ihme, The role of preferential evaporation on the ignition of multicomponent fuels in a homogeneous spray/air mixture, Proceedings of the Combustion Institute 36 (2017) 2483-2491.

[29] S.H. Won, F.M. Haas, A. Tekawade, G. Kosiba, M.A. Oehlschlaeger, S. Dooley, F.L. Dryer, Combustion characteristics of C4 iso-alkane oligomers: Experimental characterization of iso-dodecane as a jet fuel surrogate component, Combust. Flame 165 (2016) 137-143.

[30] D.J. Luning Prak, M.H. Jones, P. Trulove, A.M. McDaniel, T. Dickerson, J.S. Cowart, Physical and Chemical Analysis of Alcohol-to-Jet (ATJ) Fuel and Development of Surrogate Fuel Mixtures, Energy Fuels 29 (2015) 3760-3769.

[31] J.T. Edwards, Reference Jet Fuels for Combustion Testing, 55th AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics2017.

[32] J.M. Cohen, T.J. Rosfjord, Influences on the Sprays Formed by High-Shear Fuel Nozzle/S wirler Assemblies, J. Propul. Power 9 (1993) 16-27.

[33] C. Foley, I. Chterev, B. Noble, J. Seitzman, T. Lieuwen, Shear layer flame stabilization sensitivities in a swirling flow, International Journal of Spray and Combustion Dynamics 9 (2017) 3-18.

[34] ASTM D86-16a, Standard Test Method for Distillation of Petroleum Products and Liquid Fuels at Atmospheric Pressure, ASTM International, 2016.

[35] ASTM D6890, Test Method for Determination of Ignition Delay and Derived Cetane Number (DCN) of Diesel Fuel Oils by Combustion in a Constant Volume Chamber, ASTM International, 2012.

[36] T.J. Bruno, Improvements in the Measurement of Distillation Curves. 1. A Composition-Explicit Approach†, Ind. Eng. Chem. Res. 45 (2006) 4371-4380.

[37] T.J. Bruno, L.S. Ott, B.L. Smith, T.M. Lovestead, Complex Fluid Analysis with the Advanced Distillation Curve Approach, Anal. Chem. 82 (2010) 777-783.

[38] P.B. Govindaraju, M. Ihme, Group contribution method for multicomponent evaporation with application to transportation fuels, Int. J. Heat Mass Transfer 102 (2016) 833-845.

[39] D. Kim, J. Martz, A. Violi, A surrogate for emulating the physical and chemical properties of conventional jet fuel, Combust. Flame 161 (2014) 1489-1498.

[40] C. Ji, E. Dames, Y.L. Wang, H. Wang, F.N. Egolfopoulos, Propagation and extinction of premixed C5–C12 n-alkane flames, Combust. Flame 157 (2010) 277-287.

[41] C. Ji, S.M. Sarathy, P.S. Veloo, C.K. Westbrook, F.N. Egolfopoulos, Effects of fuel branching on the propagation of octane isomers flames, Combust. Flame 159 (2012) 1426-1436.

[42] S.H. Won, S. Dooley, F.L. Dryer, Y. Ju, A radical index for the determination of the chemical kinetic contribution to diffusion flame extinction of large hydrocarbon fuels, Combust. Flame 159 (2012) 541-551.

[43] K. Kumar, C.-J. Sung, Flame Propagation and Extinction Characteristics of Neat Surrogate Fuel Components, Energy Fuels 24 (2010) 3840-3849.

[44] K. Dussan, S.H. Won, A. Ure, F.L. Dryer, S. Dooley, Chemical Functional Group Descriptor for Ignition Propensity of Large Hydrocarbon Liquid Fuels, Proceedings of the Combustion Institute, (2018) in press.

[45] R.D. Stachler, J.S. Heyne, S. Stouffer, J.D. Miller, M. Roquemore, Investigation of Combustion Emissions from Conventional and Alternative Aviation Fuels in a Well-Stirred Reactor, 55th AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics2017.

Figure Captions

Figure 1. Comparison of representative chemical and physical properties (DCN vs. viscosity at -20 °C) of petroleum-derived jet fuels, alternative jet fuels and their blends [11]. Variabilities of Jet-A, JP-8, and JP-5 are from [23].

Figure 2. Schematic of GIT test rig for LBO experiment. Details of GIT test rig can be found in [15].

Figure 3. Distillation characteristics of Jet-A POSF 10325 determined by the boiling temperature as a function of liquid volume recovered by ASTM D86 method. Insets are direct photo of five distillation cuts collected for each of 20% liquid volume samples.

Figure 4. Relation of the equivalence ratios at LBO and measured bulkhead temperatures for (a) Jet-A POSF 10325, (b) JP-5 POSF 10289, (c) n-dodecane, and (d) Gevo-ATJ at three different air inlet temperatures (300, 450, and 550 K). Red and blue arrow bars indicate wide and narrow ranges of bulk head temperature and LBO data for statistical analyses, respectively.

Figure 5. Comparison of the measured equivalence ratio at LBO as a function of air inlet temperature for Jet-A POSF 10325 and JP-5 POSF 10289 fuels.

Figure 6. The measured DCN values of five distillation cuts (20 % liquid volume fraction each) for Jet-A POSF 10325 and JP-5 POSF 10289 fuels.

Figure 7. Comparison of the equivalence ratios at LBO for n-dodecane and Gevo-ATJ POSF 10151 as a function of air inlet temperature.

Figure 8. The measured DCN values for five distillation cuts (20 % liquid volume fraction each) of Jet-A POSF 10325, compared to the estimated DCN values of Surrogates 1 and 2 previously reported in [22]. Error bars in DCN estimation are from the uncertainty evaluated from regression analysis.

Figure 9. Comparison of the normalized equivalence ratio at LBO for Jet-A, surrogate 1, and surrogate 2 at three different air inlet temperatures.

Figure 10. Relationship between the measured equivalence ratio at LBO and (a) DCN of whole fuel sample, and (b) DCN of initial distillation cut (20 % liquid volume) of each fuel, indicative of the impact of preferential vaporization on LBO.

Table Captions

Table 1. Summary of selected fuel properties for Jet-A POSF 10325 and JP-5 POSF 10289; Derived cetane number (DCN), hydrogen to carbon molar ratio (H/C ratio), average molecular weight (MW), threshold sooting index (TSI), liquid density at 15 °C, viscosity at -20°C, and ASTM D86 distillation results.

Table 2. Summary of selected fuel properties for n-dodecane and Gevo-ATJ fuels; Derived cetane number (DCN), hydrogen to carbon molar ratio (H/C ratio), average molecular weight (MW), threshold sooting index (TSI), liquid density at 15 °C, viscosity at -20 °C, and ASTM D86 distillation results *Boiling temperature of n-dodecane.

Table 3. Summary of composition for surrogates 1 and 2 [22] and comparison of Combustion Property Targets for Jet-A POSF 10325 and both surrogates; Derived cetane number (DCN), hydrogen to carbon molar ratio (H/C ratio), average molecular weight (MW), threshold sooting index (TSI), and liquid density at 15 °C, as well as ASTM D86 distillation measurements (from AFRL).

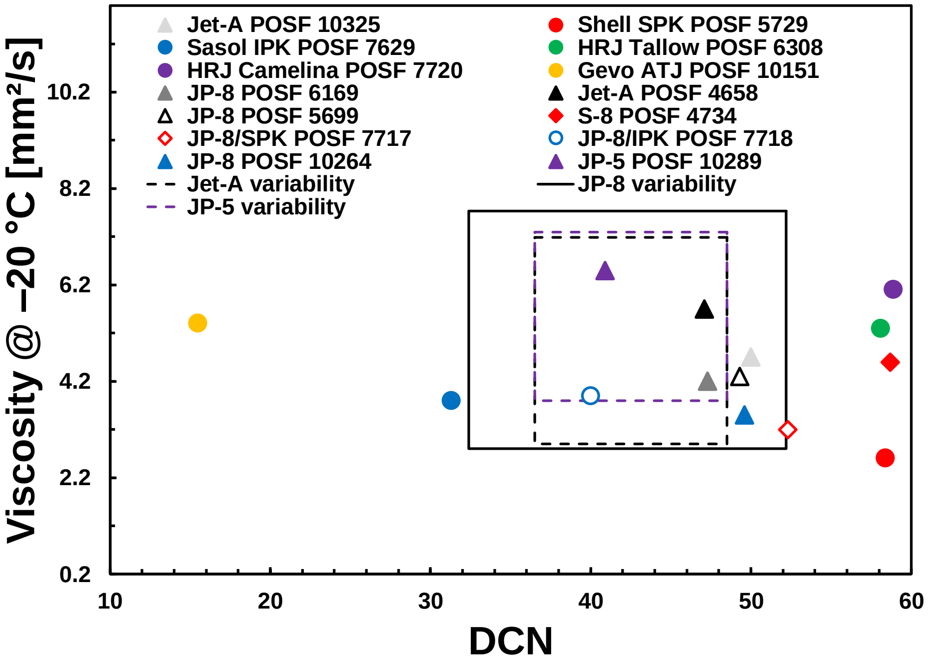

Jet-A POSF 10325
Sasol IPK POSF 7629
HRJ Camelina POSF 7720
JP-8 POSF 6169
JP-8 POSF 5699
JP-8/SPK POSF 7717
JP-8 POSF 10264
Jet-A variability
JP-5 variability
Shell SPK POSF 5729
HRJ Tallow POSF 6308
Gevo ATJ POSF 10151
Jet-A POSF 4658
S-8 POSF 4734
JP-8/IPK POSF 7718
JP-5 POSF 10289
JP-8 variability
Viscosity @ −20 °C [mm²/s]
10.2
8.2
6.2
4.2
2.2
0.2
10
20
30
40
50
60
DCN

Figure 1

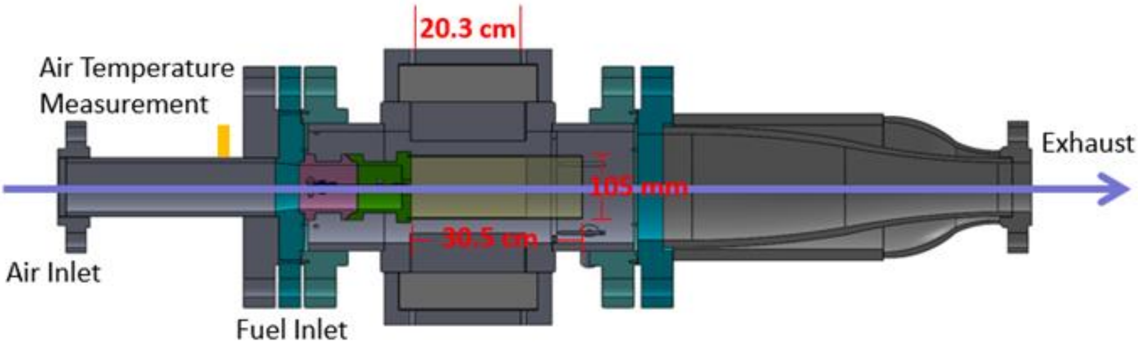

20.3 cm
Air Temperature Measurement
Exhaust
105 mm
30.5 cm
Air Inlet
Fuel Inlet

Figure 2

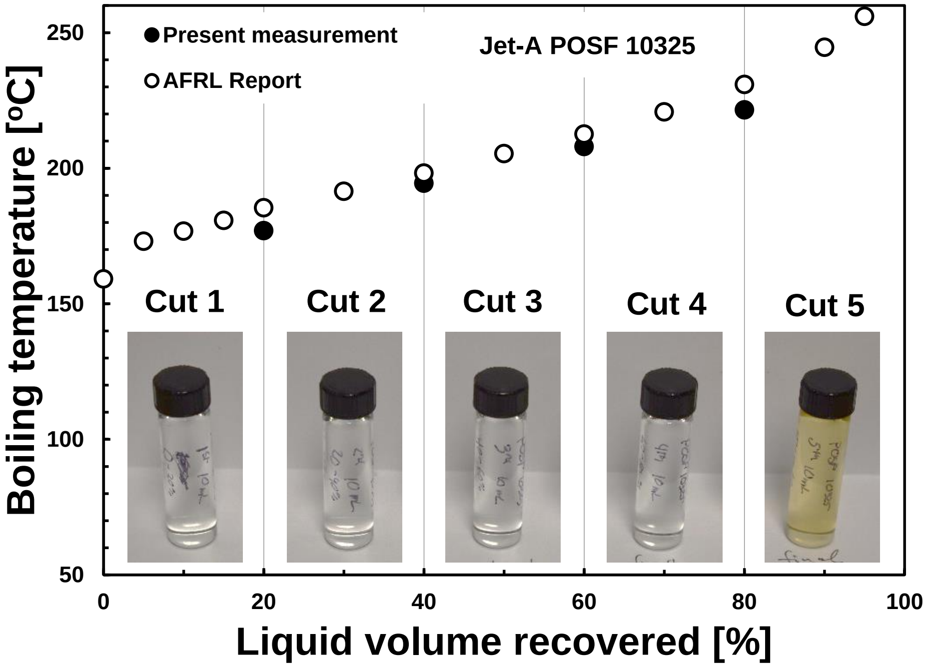

● Present measurement
○ AFRL Report
Jet-A POSF 10325
Cut 1
Cut 2
Cut 3
Cut 4
Cut 5
250
200
150
100
50
0
20
40
60
80
100
Boiling temperature [°C]
Liquid volume recovered [%]

Figure 3

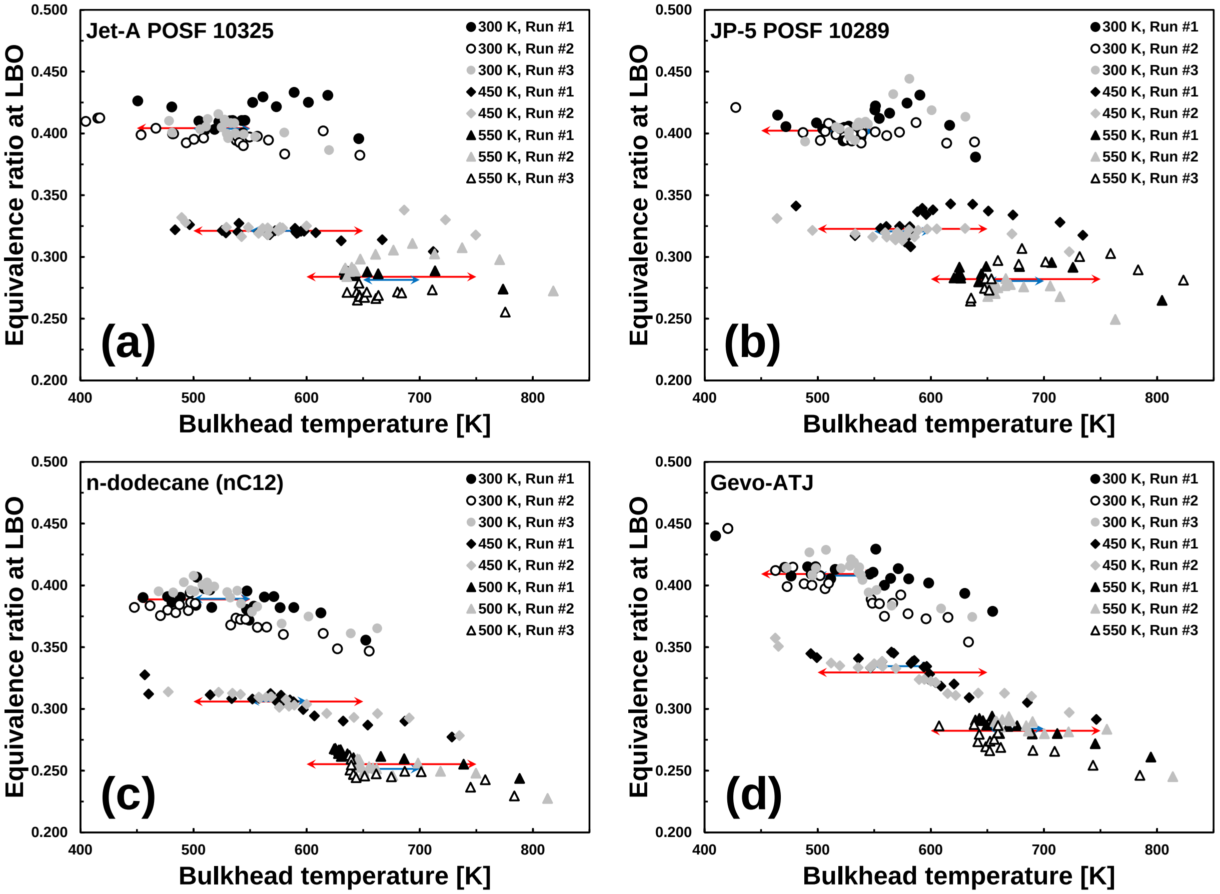

Jet-A POSF 10325
(a)
JP-5 POSF 10289
(b)
n-dodecane (nC12)
(c)
Gevo-ATJ
(d)
300 K, Run #1
300 K, Run #2
300 K, Run #3
450 K, Run #1
450 K, Run #2
550 K, Run #1
550 K, Run #2
550 K, Run #3
500 K, Run #1
500 K, Run #2
500 K, Run #3
Equivalence ratio at LBO
Bulkhead temperature [K]
0.200
0.250
0.300
0.350
0.400
0.450
0.500
400
500
600
700
800

Figure 4

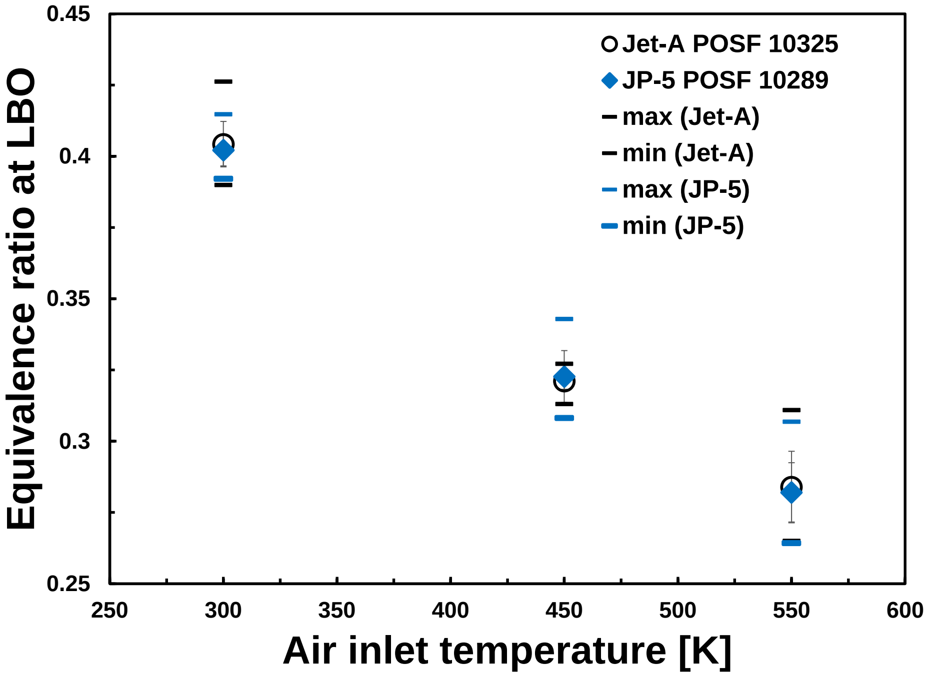
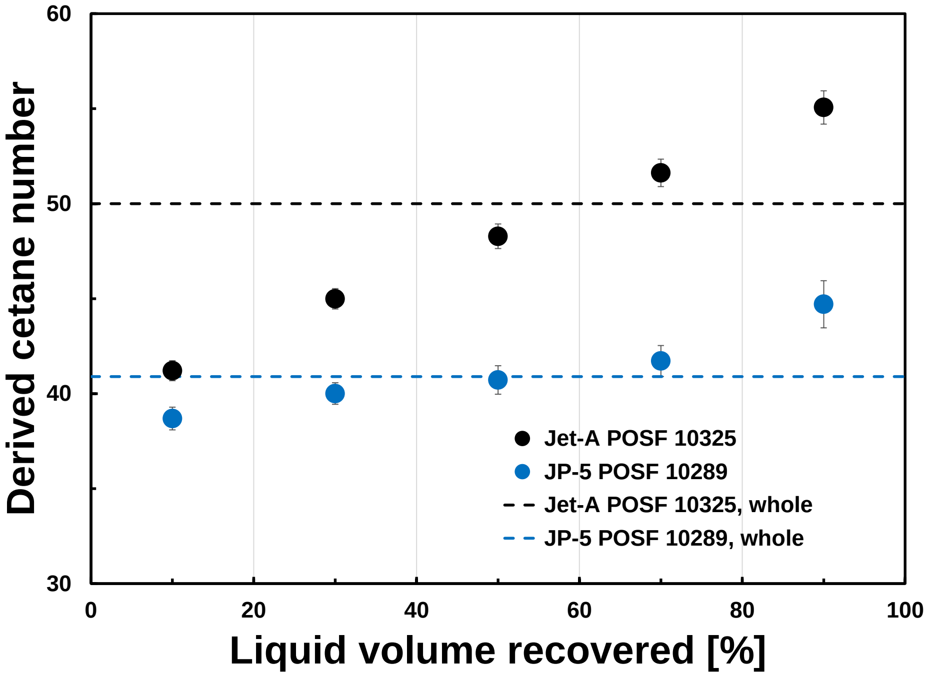

Equivalence ratio at LBO
0.45
0.4
0.35
0.3
0.25
250
300
350
400
450
500
550
600
Air inlet temperature [K]
Jet-A POSF 10325
JP-5 POSF 10289
max (Jet-A)
min (Jet-A)
max (JP-5)
min (JP-5)

Figure 5



60
50
40
30
Derived cetane number
0
20
40
60
80
100
Liquid volume recovered [%]
Jet-A POSF 10325
JP-5 POSF 10289
Jet-A POSF 10325, whole
JP-5 POSF 10289, whole

Figure 6

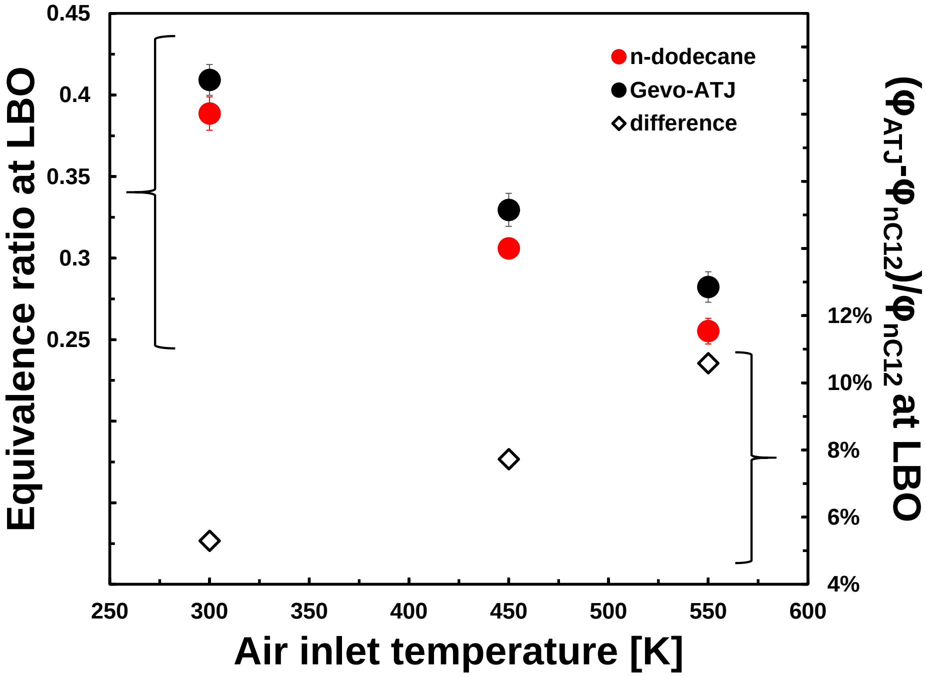
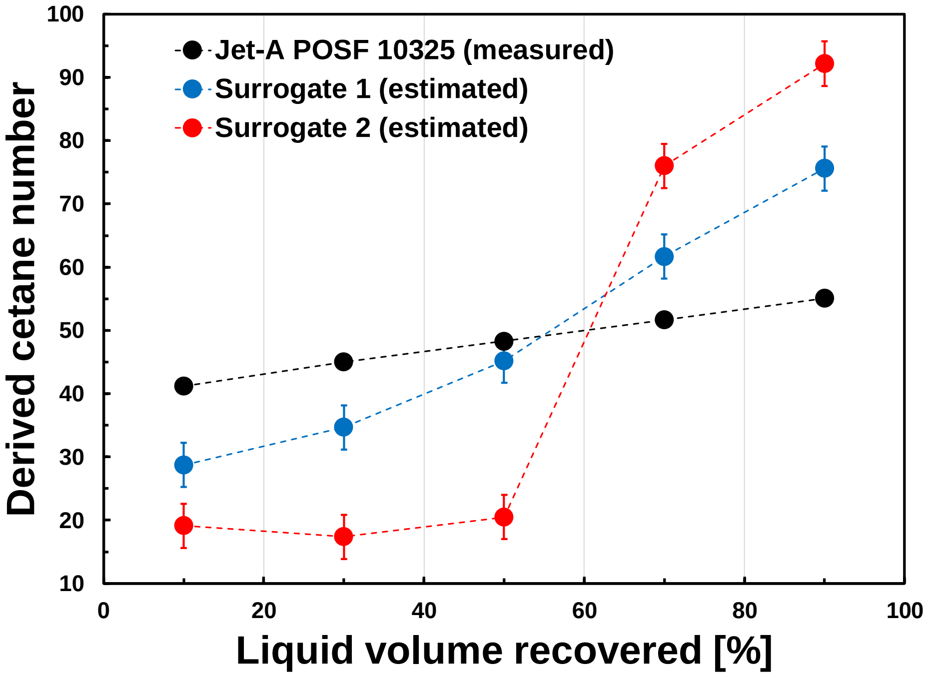

0.45
0.4
0.35
0.3
0.25
Equivalence ratio at LBO
● n-dodecane
● Gevo-ATJ
◇ difference
12%
10%
8%
6%
4%
$(\varphi_{ATJ}-\varphi_{nC12})/\varphi_{nC12}$ at LBO
250
300
350
400
450
500
550
600
Air inlet temperature [K]

Figure 7



Jet-A POSF 10325 (measured)
Surrogate 1 (estimated)
Surrogate 2 (estimated)
Derived cetane number
100
90
80
70
60
50
40
30
20
10
0
20
40
60
80
100
Liquid volume recovered [%]

Figure 8

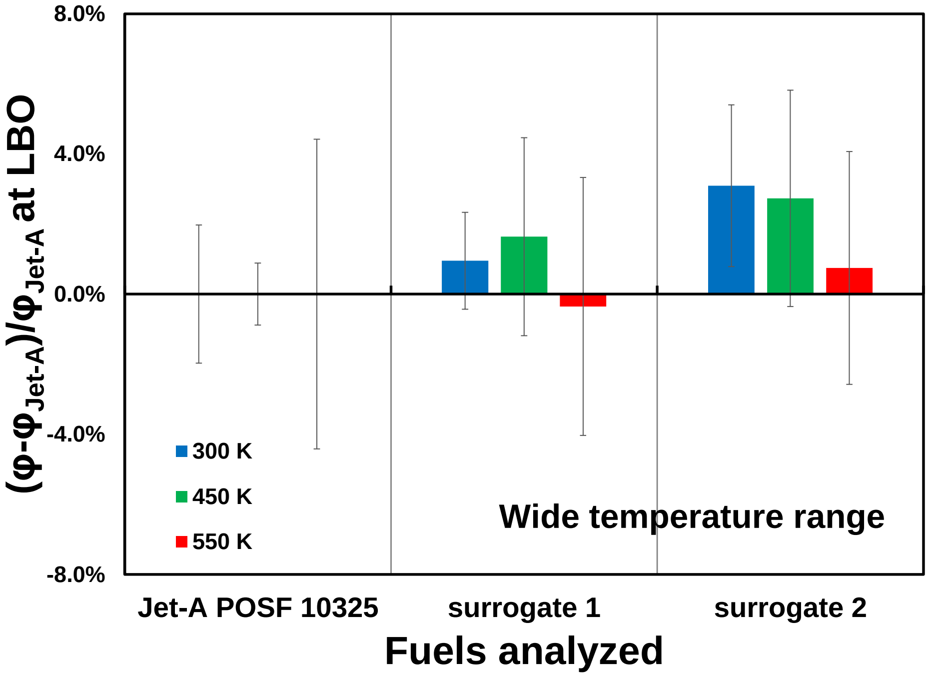
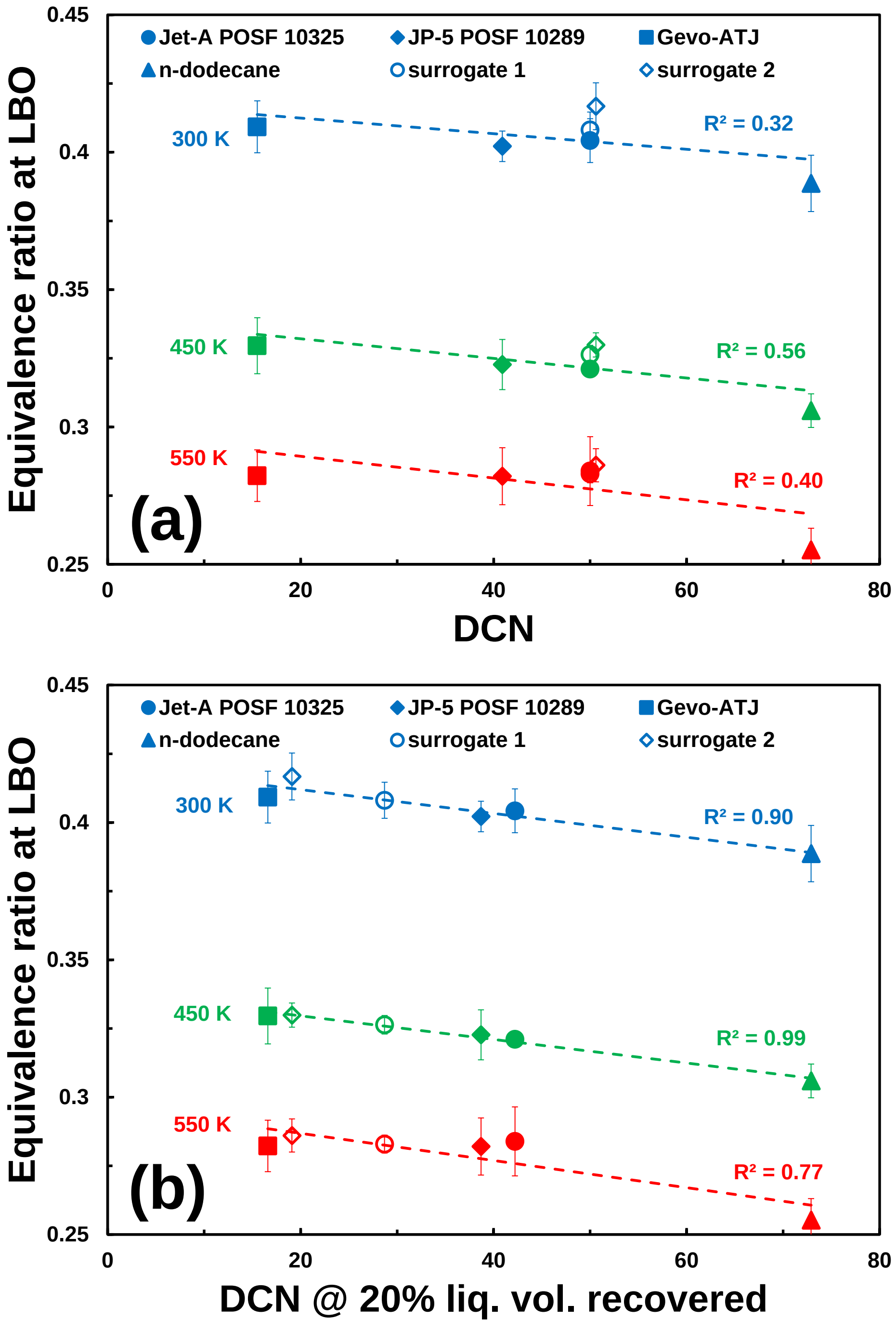

8.0%
4.0%
0.0%
-4.0%
-8.0%
(φ-φJet-A)/φJet-A at LBO
300 K
450 K
550 K
Wide temperature range
Jet-A POSF 10325
surrogate 1
surrogate 2
Fuels analyzed

Figure 9



Jet-A POSF 10325
JP-5 POSF 10289
Gevo-ATJ
n-dodecane
surrogate 1
surrogate 2
300 K
450 K
550 K
R² = 0.32
R² = 0.56
R² = 0.40
(a)
0.45
0.4
0.35
0.3
0.25
0
20
40
60
80
Equivalence ratio at LBO
DCN
Jet-A POSF 10325
JP-5 POSF 10289
Gevo-ATJ
n-dodecane
surrogate 1
surrogate 2
300 K
450 K
550 K
R² = 0.90
R² = 0.99
R² = 0.77
(b)
0.45
0.4
0.35
0.3
0.25
0
20
40
60
80
Equivalence ratio at LBO
DCN @ 20% liq. vol. recovered

Figure 10

Components	**Jet-A POSF 10325**	**JP-5 POSF 10289**
DCN	50	40.9
H/C ratio	1.961	1.868
MW [g/mol]	160.8	171.8
TSI	25.5	32.8
Density at 15 °C [kg/m^3]	803	827
Viscosity at -20°C (mm^2/s)	4.7	6.5
ASTM D86 Distillation		
10% Recovered (°C)	176	192
20% Recovered (°C)	184	199
50% Recovered (°C)	204	218
90% Recovered (°C)	245	244
End Point (°C)	269	258

Table 1

Components	**n-Dodecane**	**Gevo-ATJ**
DCN	72.9	15.5
H/C ratio	2.167	2.168
MW [g/mol]	170.3	175.6
TSI	7	15.6
Density at 15 C^{o} [kg/m^{3}]	752.6	760
Viscosity at -20^{o}C (mm^{2}/s)	4.0	5.5
ASTM D86 Distillation		
10% Recovered (°C)	217*	178
20% Recovered (°C)		179
50% Recovered (°C)		182
90% Recovered (°C)		227
End Point (°C)	217*	255

Table 2

	Target jet fuel	**Surrogate 1**	**Surrogate 2**
Components	**Jet-A POSF 10325**	**mole fraction**	**mole fraction**
n-dodecane		0.490	
n-hexadecane			0.365
iso-octane		0.210	0.310
1,3,5-trimethylbenzene		0.300	0.325
	Combustion Property Targets (CPTs)		
DCN	50	50	50.6
H/C ratio	1.961	1.961	1.947
MW [g/mol]	160.8	143.2	156.9
TSI	25.5	23.8	25.5
Density at 15 C^o [kg/m^3]	803	768	777
ASTM D86 Distillation			
10% Recovered (°C)	176	139	121
20% Recovered (°C)	184	157	131
50% Recovered (°C)	204	194	234
90% Recovered (°C)	245	212	278
End Point (°C)	269	226	281

Table 3