Abstract: A machine learning framework has been developed to predict volume swell of non-metallic materials commonly found in commercial aircraft fuel systems submerged in neat molecules. Volume swell, a material compatibility concern, serves as a significant impediment for the minimization of the environmental impact of aviation. Sustainable aviation fuels, the only near and mid-term solution to mitigating environmental impacts, are limited to low blend limits with conventional fuel due to material compatibility/O-ring swell issues. A neural network was trained to predict volume swell for neat molecules found in conventional jet fuel. Subsequent blend optimization incorporated swell predictions for cyclo- andiso-alkanes to create a high-performance jet fuel within ‘drop-in’ limits. Aircraft performance analysis was performed on a Boeing 737-800 to quantify the payload increase and fuel savings conferred by the high-performance jet fuel. Optimization considering nitrile rubber volume swell achieved median specific energy [MJ/kg] and energy density [MJ/L] increases of 1.9% and 5.1% respectively relative to Jet A, resulting in a 5.4% reduction in fuel volume and a 2.5% payload increase for a Boeing 737-800 flying from New York City to San Francisco.

Keywords: Sustainable Aviation Fuel, High-Performance Jet Fuel, Volume Swell, Aircraft Performance Analysis

1. Introduction

Although aviation currently contributes a relatively small percent of global anthropogenic CO₂ emissions at ~2% [1], air travel is expected to double by the year 2037 [2], with associated particulate matter (PM) and radiative forcing (RF) emissions nearly doubling the current climate impact of aviation transportation. This growth could make aviation transportation account for a significant fraction of total anthropogenic carbon emissions. Sustainable aviation fuel (SAF) is the only near and mid-term opportunity for the minimization of aviation emissions. Currently, SAF adaption is limited by both the approval of novel fuels and the cost of currently approved fuels. Of the five SAFs currently approved, four are limited to a max blend ratio of 50% with conventional jet fuel due to material compatibility issues (e.g., O-ring swell) [3]. Specifically, aircraft have been found to leak significant quantities of fuel over the timescale of hours when volume swell is not sufficient [4].

Aromatics provide volume swell character to conventional jet fuel but are generally undesirable due to their low energy and tendency to form soot. Prior work [5] has illuminated a novel path for the approval of SAFs beyond 50% materials compatibility. This study indicated
that blends of 30% cycloalkanes in synthetic paraffinic kerosene (SPK) exhibit volume swell properties similar to conventional jet fuel despite the lack of aromatic content. Moreover, these cycloalkane compounds have been found to increase the value of SAFs via aircraft operation improvements by increasing the fuel energy content [6].

In this study, volume swell was predicted for neat molecules via a neural network. These predictions were subsequently implemented into the optimization of high-performance jet fuels (HPFs), which represent a subset of SAFs that improves the performance of aircraft while remaining within ‘drop-in’ limits. This optimization illuminates a path for maximizing the value of SAFs by minimizing PM emissions, maximizing energy content, meeting previously reported SAF operability and safety constraints, and satisfying novel swell requirements. Subsequent aircraft performance analysis was performed using HPFs to determine fuel volume reductions and payload capacity increases achievable relative to Jet A. Combined, these results will guide current and ongoing research and development efforts of novel SAFs towards eclipsing the cost-benefit threshold of HPFs.

2. Methods / Experimental

Volume swell measurements used for this work consist of a single set of optical dilatometry measurements from literature [5]. Volume swell was measured for 10 non-metallic materials commonly found in commercial aircraft fuel systems and seven molecular groups. The materials were submerged in an aromatic-free SPK blended with neat molecules to examine the effect of the molecules on volume swell. The volume swell data was split into training and test frames. Principal component analysis (PCA) was performed on the training frame, and the resulting principal components were used to train the neural network. 10 k-fold cross-validation was used to validate the neural network. After the neural network was generated, the PCA model was applied to the test frame and volume swell predictions were made to provide additional model validation. The prediction frame consisted of 24 cyclo- and iso-alkanes that did not have volume swell data in literature but were of interest for HPF optimization. The PCA model was applied to this frame and volume swell was predicted via the neural network. Molecules that met feature importance screening criteria were subsequently incorporated into HPF optimization. The rest of this paper will focus on HPF optimization and subsequent aircraft performance analysis applied to optimized HPFs.

HPF optimization done in this study leveraged code from previous efforts [6][7]. The general approach was to use blending rules from literature coupled with ant colony optimization to maximize performance and value-added properties -specific energy (SE) [MJ/kg] and energy density (ED) [MJ/L]- for blends of molecules in the jet range while remaining within operability limits. Operability are required to ensure novel fuels have no associated deleterious risks. A total of eight operability and safety properties served as constraints for optimization: volume swell, derived cetane number (DCN), density, kinematic viscosity at -20°C, flash point, freezing point, 10% recovered temperature, and final boiling point. The result of optimization was a Pareto front indicating the best performance properties achievable via blends of molecules without violating operability limits.

Nitrile rubber volume swell values were used for optimization because of the commonality of nitrile rubber in commercial aircraft fuel systems and the low mean absolute error achieved for neural network predictions. The optimization started with 1,000 random initial guesses that met operability limits. The totality of these solutions underwent an initial optimization run, with subsequent optimization revisions guided by 2σ convergence criteria for
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\( \Delta SE \) and \( \Delta ED \) across the Pareto front. Solutions that fell outside the 2\( \sigma \) range underwent further optimization for 10 consecutive revision rounds, with \( \sigma \) here being the physical uncertainty associated with the neat molecule SE and ED values used for optimization.

Volume swell was predicted for blends of cyclo- and \( iso \)-alkanes under the assumption that their interaction effects would be sufficiently weak due to their lack of hydrogen bonding and low polarity. It follows that volume swell should vary linearly with the concentration of cyclo- and \( iso \)-alkanes within the blending limits provided in literature [5]. This assumption may not hold for aromatics because they exhibit weak dipole-dipole interactions and hydrogen bonding which can affect molecular solubility and shift equilibrium concentrations, resulting in unpredictable blending behavior. Assuming a linear correlation between volume swell and the concentration of cyclo- and \( iso \)-alkanes allowed for the creation of a blending rule:

\[
swell_{blend} = \Sigma (swell_i \times \varphi_i)
\]

where \( \varphi_i \) represents the individual volume fraction of each molecule. This blending rule was coupled into the optimization framework as a constraint.

Aircraft performance analysis was performed on a Boeing 737-800 flying 2150 nautical miles using the Environmental Design Space (EDS) [8]. A Design of Experiments was created to maximize the information learned from a computationally inexpensive number of EDS run cases. SE and density were varied from -15% to +15% of that of Jet A, while off-design mission ranges were evaluated in 500nm increments until the maximum design range and payload was reached. Performance parameters of interest were the change in fuel volume and weight as a function of SE, density, and flight range. The statistical package, JMP, was used to develop surrogate models for the aircraft performance metrics as functions of the SE, density, and flight range. Fuel volume decrease was taken as the reduction in fuel volume relative to Jet A using Equation 2.

\[
volume = \frac{weight}{\rho}
\]

Equation 3 was derived via the EDS analysis. Payload capacity increase was taken as the difference in fuel weight between the HPF and Jet A per Equation 3, where \( R \) represents the flight range.

\[
weight = 2.71 \times 10^4 + 59.64 \rho - 1.37 SE + 12.05 R + (\rho - 1.01) [-530.77(\rho - 1.01)] + (\rho - 1.01) [-1.30 \times 10^{-3} (SE - 1.88 \times 10^4)] + (SE - 1.88 \times 10^4)[1.04 \times 10^{-4}(SE - 1.88 \times 10^4)] + (\rho - 1.01)[0.278(R - 1500)] + (SE - 1.88 \times 10^4)[-8.59 \times 10^{-4}(R - 1500)] + (R - 1500)[4.06 \times 10^{-4}(R - 1500)]
\]

3. Results and Discussion

Figures 1 and 2 show the specific energy plotted against energy density with the Pareto front consisting of 7,196 optimized blends of 10 molecules. The red markers represent conventional jet fuels, which serve as the origin for the plot. Green, brown, and pink markers represent molecules used for optimization. The 2D kernel density plot represents the distribution of Jet A taken from the Petroleum Quality Information System (PQIS), a Department of Defense database dedicated to fuel quality information. The dark blue line represents the highest values from the PQIS. Fuels that exceed the SE and ED values of this line and meet operability requirements have been deemed high-performance jet fuels. The HPF region is indicated by the
yellow-purple colormap, with percent fuel reduction by volume and percent payload increase by weight relative to Jet A displayed in Figures 1 and 2 respectively.

Figure 1 (left) and Figure 2 (right). Specific energy plotted against energy density with the optimized Pareto front representing blends of cyclo- and iso-alkanes meeting nitrile rubber volume swell requirements in addition to other operability limits.

Median specific energy and energy density values across the Pareto front are 43.9 MJ/kg and 36.3 MJ/L respectively, representing 1.9% and 5.1% gains relative to Jet A. Comprehensive performance statistics across the Pareto front are displayed in Table 1. The Pareto front is fairly constrained relative to previous optimization efforts which spanned the majority of the density region represented by the straight blue lines. The Pareto front is limited on the right because it cannot achieve a higher specific energy than the set of molecules used for optimization. Specifically, the highest specific energy was that of cis-1,2-dimethylcyclooctane and farnesane at 43.95 MJ/kg. The Pareto front is constrained on the left because it violates the upper density limit. The Pareto front does not appear to reach the upper density limit in Figures 1 and 2 because ASTM D1298 reproducibility uncertainty is incorporated into the optimization constraints to provide a factor of safety.

Median Pareto front SE and ED increases correspond to a 5.4%/857L decrease in required fuel and an 2.5%/315kg increase in payload capacity. The increased payload capacity can add roughly five passengers per flight. In general, fuel volume reduction increases with increasing ED. Volume reductions from increasing SE were negated by decreasing density per Equation 2. Payload increases correlate strongly with increasing SE, with higher ED values reducing the payload capacity due to increased density per Equation 3. In general, percent fuel reduction and percent payload capacity increase with longer range.

<table>
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<th>Property</th>
<th>Min</th>
<th>Median</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>SE [%]/[MJ/kg]</td>
<td>1.76/43.82</td>
<td>1.94/43.90</td>
<td>2.02/43.93</td>
</tr>
<tr>
<td>ED [%]/[MJ/L]</td>
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<td>5.11/36.34</td>
<td>5.61/36.52</td>
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<tr>
<td>Fuel Reduction [%]/[L]</td>
<td>4.75/752.6</td>
<td>5.41/857.2</td>
<td>5.88/932.0</td>
</tr>
<tr>
<td>Payload Increase [%]/[kg]</td>
<td>2.25/286.7</td>
<td>2.48/315.3</td>
<td>2.56/326.7</td>
</tr>
</tbody>
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Compositions and functional groups for solutions across the Pareto front can be seen in Figure 3, with blue lines representing mean blend values. Solutions consisted primarily of monocycloalkanes blended with either dicycloalkanes or farnesane, with a critical point existing
at 43.91 MJ/kg. Despite its low volume swell, farnesane appeared in solutions toward the right of the Pareto front because of its high SE. Amongst dicycloalkanes, cis-decalin was favored, likely because of its low freezing point and higher DCN than trans-decalin. Amongst monocycloalkanes, cis-1,2-dimethylcyclooctane was favored despite having a high viscosity and low DCN because of its high SE and ED.

Figure 3 (left). Composition and functional groups of solutions across the HPF Pareto front.

Figure 4 (right). Operability/safety properties of solutions across the HPF Pareto front.

Operability and safety properties of solutions across the Pareto front can be seen in Figure 4, with dashed lines representing operability limits. Volume swell did not serve to constrain optimization, with the lowest volume swell solutions occurring where the concentration of farnesane was the highest. The minimum volume swell value was 5.5%, well above the 3.7% v/v lower limit for nitrile rubber. DCN remained consistent across the Pareto front, with a standard deviation of 0.008. Molecules with low DCN values, such as methylcyclohexane and trans-decalin, were generally avoided. Density served to bound the left of the Pareto front, hindering the addition of more dicycloalkanes. It scaled with volume swell, decreasing linearly as dicycloalkanes were replaced by monocycloalkanes and as farnesane was added. Viscosity remained close to its upper limit, indicating that it was a limiting constraint. This is likely because of the high viscosity of cis-1,2-dimethylcyclooctane, which was favored across solutions. Flash point remained well above its limit of 38°C, decreasing as dicycloalkanes were removed and subsequently increasing as farnesane was added. Freezing point decreased between 43.90 and 43.91 MJ/kg due to the addition of light monocycloalkanes and increased as farnesane was added from 43.91 to 43.93 MJ/kg. The 10% recovered temperature remained well below its limit, increasing as sec-butyldecalin and subsequently farnesane were added. The final boiling point also remained well below its limit, following a stepwise pattern because it was determined by the highest boiling point molecule in the solutions. Molecules that determined final boiling points across the Pareto front were sec-butyldecalin, heptylcyclohexane, and farnesane from left to right. High boiling points could serve as an impediment to the use of large cyclo- and iso-alkanes.
4. Conclusions

A framework has been developed to predict volume swell of non-metallic materials commonly found in commercial aircraft fuel systems due to neat molecules and subsequently optimize blends of molecules that swell within the range of conventional jet fuel. This study indicates that cycloalkanes are a suitable replacement for aromatics considering volume swell requirements. Optimized solutions achieved a median nitrile rubber volume swell of 6.2% v/v, well above the 3.7% v/v lower limit. The emissions reduction from replacing aromatics with cycloalkanes would be significant: cycloalkanes produce 88% less soot on average compared to aromatics [9]. It is estimated that direct radiative forcing from aviation-related soot emissions is ~9.5 mW/m² [10], approximately 12% of the total RF associated with aviation [11]. It follows that the replacement of aromatics with cycloalkanes could reduce RF associated with aviation by roughly 10.6%. Value and performance gains are also conferred by replacing aromatics; median specific energy and energy density gains of 1.9% and 5.1% were achieved in this study, which can decrease fuel requirements by 5.4% or increase payload capacity by 2.5%, conferring environmental and monetary benefits to airlines.

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6. References