



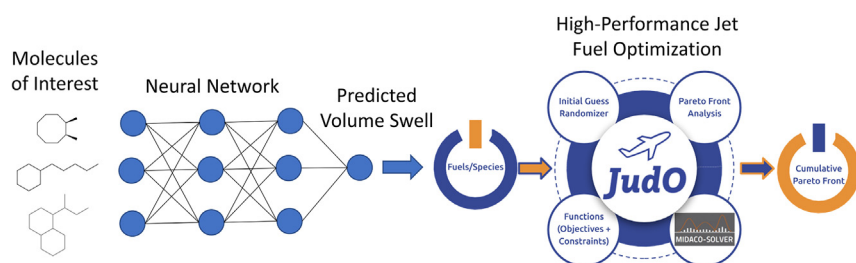
A machine learning framework for drop-in volume swell characteristics of sustainable aviation fuel

Shane Kosir^{a,*}, Joshua Heyne^a, John Graham^b

^a University of Dayton, Department of Mechanical & Aerospace Engineering, 300 College Park, Dayton, OH 45469, United States

^b University of Dayton Research Institute, Nonstructural Materials Division, 300 College Park, Dayton, OH 45469, United States

GRAPHICAL ABSTRACT



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ABSTRACT

A machine learning framework has been developed to predict volume swell for 10 non-metallic materials submerged in neat compounds. The non-metallic materials included nitrile rubber, extracted nitrile rubber, fluorosilicone, low temp fluorocarbon, lightweight polysulfide, polythioether, epoxy (0.2 mm), epoxy (0.04 mm), nylon, and Kapton. Volume swell, a material compatibility concern, serves as a significant impediment for the minimization of the greenhouse gas emissions of aviation. Sustainable aviation fuels, the only near and mid-term solution to mitigating greenhouse gas emissions, are limited to low blend limits with conventional fuel due to material compatibility issues (i.e. O-ring swell). A neural network was trained to predict volume swell for non-metallic materials submerged in neat compounds. Subsequent blend optimization incorporated nitrile rubber volume swell predictions for iso- and cycloalkanes to create a high-performance jet fuel within 'drop-in' limits.

The results of this study are volume swell predictions for 3 of the 10 materials -nitrile rubber, extracted nitrile rubber, and polythioether- with holdout errors of 12.4% or better relative to mean volume swell values. Optimization considering nitrile rubber volume swell achieved median specific energy [MJ/kg] and energy density [MJ/L] increases of 1.9% and 5.1% relative to conventional jet fuel and an average volume swell of 6.2% v/v which is within the range of conventional fuels. Optimized solutions were heavily biased toward mono-cycloalkanes, indicating that they are a suitable replacement for aromatics. This study concludes that cycloalkanes can replace aromatics in jet fuel considering volume swell and other operability requirements while significantly reducing soot and particulate matter emissions.

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

* Corresponding author.

E-mail address: kosirs1@udayton.edu (S. Kosir).

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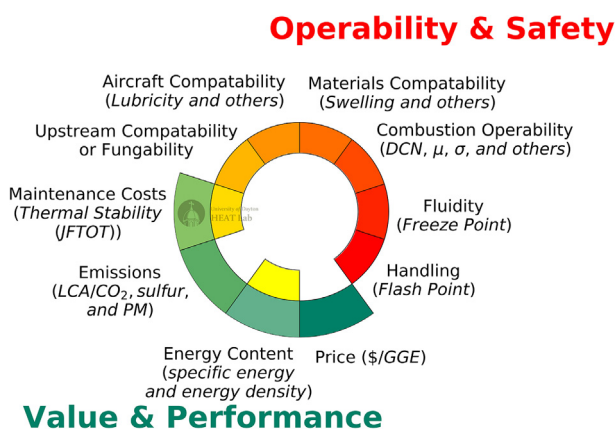


Fig. 1. Operability and safety constraints that need to be met for SAF approval (autumn colormap) and opportunities to improve the value and performance of a SAF (green colormap). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

climate impact of aviation transportation. This growth, combined with terrestrial electrification and recent International Maritime Organization (IMO) regulations [3], 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 greenhouse gas emissions. Currently, SAF adaption is limited by both the approval of novel fuels and the cost of currently approved fuels. Fig. 1 illustrates operability and safety constraints that need to be met for a novel SAF to be approved in the autumn colormap. Opportunities to improve the value and performance of a SAF are illuminated in the green colormap. 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 (i.e., O-ring swell) [4]. Specifically, aircraft have been found to leak significant quantities of fuel over the timescale of hours when volume swell is not sufficient [5].

Aromatics provide the majority of volume swell character to conventional jet fuel but are generally undesirable due to their low specific energy (SE) and tendency to form soot. Prior work [6] 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, as can be seen in Fig. 2. The dashed lines in the figure represent the lower volume swell limits of 12 conventional fuels. Many cycloalkanes are close to or exceed the lower limits, indicating that they can confer similar volume swell to a low-aromatic Jet A. It is expected that higher concentrations of cycloalkanes would confer further volume swell benefits as can be seen in Fig. 8. Moreover, these cycloalkane compounds have been found to increase the value of SAFs via aircraft operation improvements by increasing the fuel energy content [7].

Here, it is proposed that cycloalkanes be used in SAFs to (1) overcome the blend limit of SAFs, (2) minimize PM and RF of aviation emissions, and (3) add to the value proposition of SAFs. A machine learning framework has been developed to achieve equivalent volume swell by replacing aromatics with cycloalkanes. Volume swell was first predicted for 10 non-metallic materials submerged in neat compounds via a neural network. Volume swell predictions for nitrile rubber were subsequently implemented into the optimization of high-performance fuels (HPFs) via ant colony optimization. The result was a HPF, which represents 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.

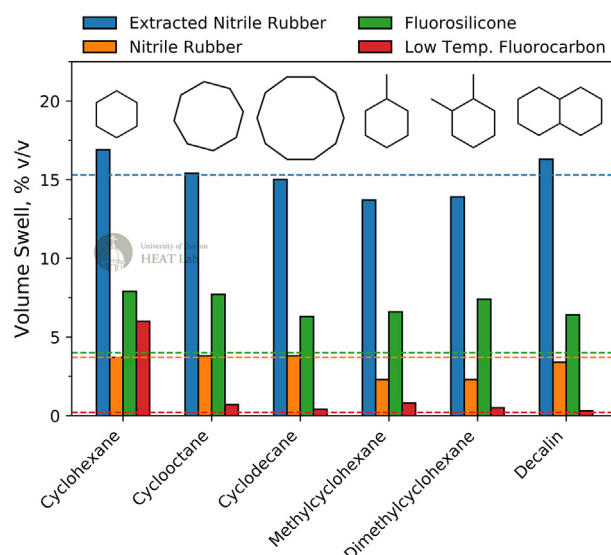


Fig. 2. Volume swell of four O-ring materials in cycloalkanes blended at 30% v/v with zero-aromatic SPK. Dashed lines represent conventional jet fuel lower limits, which many cycloalkanes exceed.

Combined, these results will guide current and ongoing research and development efforts of HPFs towards eclipsing the cost-benefit threshold of SAFs.

To date, volume swell predictions remain fairly scarce in literature. They generally fall into two categories: statistical approaches, such as that of Graham et al. [8], and ab initio calculations to determine fuel-polymer interaction energies [9–11]. Graham et al. developed a method of statistically comparing the swell behavior of alternative jet fuels (AJFs) to a reference set of JP-8 fuels. Specifically, the overlap in the volume swell 90% prediction intervals between the AJFs and the JP-8s served as an indicator of the compatibility between the fuels. This work extends that done by Graham et al. to neat compounds and allows for the determination of explicit volume swell values which can be used for HPF optimization, surrogate generation, and AJF prescreening.

2. Material and methods

2.1. Material

Volume swell measurements used for this work consist of a single set of optical dilatometry measurements from literature [6]. Volume swell was measured for 10 non-metallic materials submerged in compounds from seven groups. The non-metallic materials, which are all common in commercial aircraft fuel systems, included nitrile rubber, extracted nitrile rubber, fluorosilicone, low temp fluorocarbon, lightweight polysulfide, polythioether, epoxy (0.2 mm), epoxy (0.04 mm), nylon, and Kapton. Each material had volume swell measurements for one *iso*-alkane, 10 monocycloalkanes, one dicycloalkane, six alkyl-aromatics, one diaromatic, three cycloaromatics, and one diamondoid, with a total of 230 observations. The materials were submerged in an aromatic-free SPK blended with neat compounds to examine the effect of the compounds on volume swell.

2.2. Methods

Fig. 3 depicts the methodology used to train a neural network to predict volume swell for neat compounds. The volume swell data was split into *training* (blue) and *test* (green) frames. Principal component analysis (PCA) was performed on the training frame, and the resulting principal components (PCs) were used to train the neural network. 10 k-fold cross-validation was used to validate the neural network.

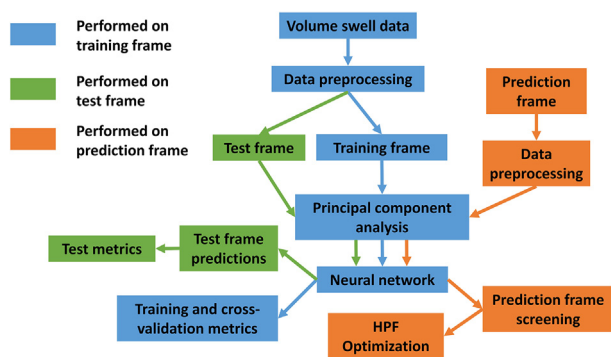


Fig. 3. Flowchart for neural network training.

After the neural network was generated, the PCA model was applied to the test frame and volume swell predictions were made to provide holdout validation.

The *prediction frame* (orange) consisted of 24 *iso*- and cycloalkanes 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. Compounds that met feature importance screening criteria were subsequently incorporated into HPF optimization, which can be seen in Fig. 4. Neat compound properties used for HPF optimization can be seen in the [Supplementary Material](#).

2.2.1. Data preprocessing

Volume swell data for blends of SPK and neat compounds was linearly extrapolated to a concentration of 100% to estimate the volume swell of the neat compounds. This was done to provide a common basis to compare volume swell observations with varying ratios of SPK and neat compounds. The assumption for extrapolation was that volume swell would be consistent with the hydrocarbon concentration within the blending limits provided in literature (i.e. 30% v/v) [6].

Previous work [6] determined that molar volume was the primary factor influencing volume swell in the cycloalkanes, with lower molar volume resulting in higher volume swell due to increased ease of absorption of smaller compounds into non-metallic materials. Additional selectivity occurred for some non-metallic materials, including nitrile rubber, polysulfide, and polythioether, due to variations in compound structure such as substitution position and ring size. It follows that molar volume, compound structure, and non-metallic material served as training features for the neural network.

Compound structure descriptors used to train the neural network were generated using RDKit [12], an open-source Python toolkit for cheminformatics. A total of 27 features were used for model training,

Table 1
Distribution of select features used to train the neural network.

Feature	Min Value	Median Value	Max Value	Standard Deviation
Molar volume, mL/mol	108.7	140.0	275.9	37.2
-CH ₃ (linear)	0	1	5	1.3
-CH ₂ - (linear)	0	0	7	2.0
> CH- (linear)	0	0	3	0.6
-CH ₂ - (cycloalkane ring)	0	4	12	3.6
> CH- (cycloalkane ring)	0	0	4	1.2
=CH- (aromatic ring)	0	0	8	2.4
=C < (aromatic ring)	0	0	3	1.1

with the distribution of select features shown in Table 1. The entirety of the training features, including material type and additional compound structure, can be seen in the [Supplementary Material](#). Features with fewer than 10% distinct values were deemed redundant and removed. The data was split into training and test frames by randomly down-selecting four compounds from each material, resulting in a 83/17% split.

2.2.2. Principal component analysis

Principal component analysis was used to reduce the dimensionality of the training data and to weaken correlations between features. PCA involves combining potentially correlated features into linearly uncorrelated variables called principal components. The PCA model was generated using the open-source machine learning platform H₂O Flow [13]. Data was standardized prior to performing PCA to avoid biasing features with large magnitudes. The GramSVD PCA method was used, which computes a Gramian matrix with the data and subsequently performs singular value decomposition using the Java Matrix package [14]. The result is a matrix containing the eigenvectors associated with each PC.

2.2.3. Neural network training

The training frame was used to develop a neural network in H₂O Flow with auto machine learning (AutoML) used to optimize hyperparameters. 22 of the 27 principal components were used to train the model, encompassing 100% of the variance in the training frame. A preset grid of neural networks were trained and scored, followed by random generation of neural networks that proceeded to train for five hours. During AutoML, weights were initialized by the uniform adaptive methodology [15], which optimizes initial weights based on the size of the network. An adaptive learning rate was facilitated via the AdaDelta algorithm [16]. Backpropagation was performed for cross-validation models followed by stochastic gradient descent until the mean residual deviance of cross-validated predictions did not improve. Neural network feature importances were calculated via the Gedeon method [17], which considers the magnitude of the weights in the first two hidden layers associated with each feature.

2.2.4. Principal component screening

Compounds in the prediction frame were screened via neural network feature importances before coupling their predicted volume swell values into HPF optimization. The rationale for this screening is that neural networks cannot extrapolate outside the range of training features due to their black box nature [18]. Maximum and minimum values for each PC in the training frame bounded the screening. PCs were ordered by feature importance and a threshold of 90% cumulative feature importance was used. Compounds in the prediction frame that had PCs out of range before eclipsing the threshold were not used for HPF optimization.

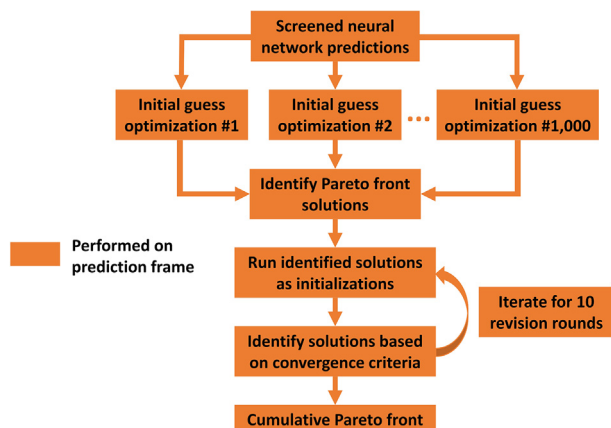


Fig. 4. Flowchart for HPF optimization.

Table 2
Neural network prediction metrics for select materials.

Material	Mean Extrapolated Neat Volume Swell, %v/v	Train MAE, % v/v	Validate MAE, % v/v	Test MAE, % v/v
Extracted Nitrile Rubber	50.5	3.9	8.8	5.3
Nitrile Rubber	28.2	2.0	3.8	3.5
Fluorosilicone	14.1	1.3	11.7	7.4
Low Temp Fluorocarbon	4.5	0.6	3.0	0.9
Lightweight Polysulfide	10.7	0.8	4.3	2.5
Polythioether	24.7	1.1	7.2	2.9

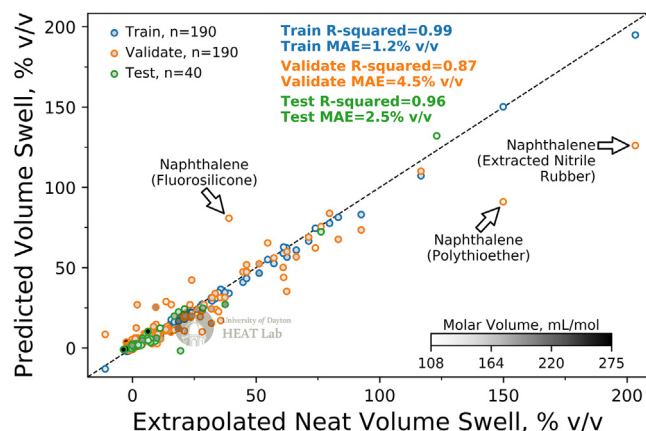


Fig. 5. Neural network train, validate, and test predictions plotted against extrapolated neat volume swell.

2.2.5. High-Performance Fuel (HPF) optimization

HPF optimization done in this study leveraged code from previous efforts [7,19]. The general approach was to use blending rules from literature coupled with ant colony optimization to maximize performance and value-added properties -SE and energy density (ED)- for blends of compounds in the jet range while remaining within operability and safety limits, see Fig. 1. Operability and safety limits are required to ensure novel fuels have no associated deleterious risks. Some examples are viscosity, which is important for fuel flow, and derived cetane number (DCN), which is important for lean blowout stability [20]. A total of eight operability and safety properties served as constraints for optimization: volume swell, DCN, density, kinematic viscosity at $-20\text{ }^{\circ}\text{C}$, 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 compounds 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 MAE achieved for neural network predictions as depicted in Table 2. The optimization started with 1000 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 ΔSE and ΔED across the Pareto front. Solutions that fell outside the 2σ range underwent further optimization for 10 consecutive revision rounds, with σ here being the physical uncertainty associated with the neat compound SE and ED values used for optimization.

3. Calculation

Volume swell was predicted for blends of cycloalkanes 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 iso- and cycloalkanes within the blending limits provided in literature. This assumption may not hold for aromatics because they

exhibit weak dipole-dipole interactions and hydrogen bonding which can affect compound solubility and shift equilibrium concentrations, resulting in unpredictable blending behavior. Assuming a linear correlation between volume swell and the concentration of iso- and cycloalkanes allowed for the creation of a blending rule:

$$\text{swell}_{\text{blend}} = \sum (\text{swell}_i \times \varphi_i) \quad (1)$$

where φ_i represents the volume fraction of compound i . This blending rule was coupled into the optimization framework as a constraint.

4. Results and discussion

The result of AutoML hyperparameter optimization and subsequent parameter tuning was a deep learning neural network consisting of two hidden layers with 500 neurons each. Rectifier activation was used for the hidden layers with a hidden dropout ratio of 0.4 for regularization. Mean learning rates were 0.143, 0.333, and 0.005 for hidden and output layers respectively. An average value of 720 epochs, taken from all 10 cross-validation models, was used for the main model.

4.1. Neural network predictions

Fig. 5 shows predictions from the train, validation, and test frames, with prediction metrics for select materials displayed in Table 2. Prediction metrics for all material groups can be seen in the Supplementary Material. The model predicts the training frame well with an R-squared of 0.99 and a mean absolute error (MAE) of 1.2% v/v. Cross-validated predictions have a R-squared and MAE of 0.87 and 4.5% v/v respectively, suggesting that a degree of overfitting is occurring. Naphthalene was a significant outlier that affected the validation prediction metrics. This is likely because naphthalene exhibits the highest degree of hydrogen bonding of compounds in the training frame, which was not a feature used to train the neural network. With the exception of naphthalene, compounds with high volume swell values had low relative prediction errors.

Prediction metrics for test predictions are intermediate to training and validation prediction metrics, with an R-squared and MAE of 0.96 and 2.5% v/v respectively. Because the test frame was not seen by the model during training, it is likely a better indicator of its generalizability. It is possible that models trained with only 90% of the training frame for 10 k-fold cross-validation resulted in reduced model performance and overestimation of the prediction error for the validation frame. Regardless, the worst-case MAE of 4.5% v/v is suitable for engineering calculations, especially for materials with higher mean volume swell such as nitrile rubber and polythioether.

Material prediction metrics are generally in agreement with observations from literature [6]. The most accurate predictions - nitrile rubber, extracted nitrile rubber, lightweight polysulfide, and polythioether- likely had low error because they exhibit selectivity based on compound structure. Specifically, volume swell showed a decreasing trend with substitution length for these materials. Additionally, 1,2-dimethylcyclohexane was the preferred substitution pattern for these materials with the exception of lightweight polysulfide. Fluorosilicone, which swelled significantly when submerged in the cycloalkanes and followed the trend previously described with substitution length, had

low prediction accuracy. This is possibly because fluorosilicone did not follow the trend of 1,2-dimethylcyclohexane being the preferred substitution pattern. Low temp fluorocarbon had poor accuracy, possibly because it was weakly responsive when submerged in the cycloalkanes and only slightly followed the trend with substitution length. The epoxies, nylon, and Kapton had poor prediction metrics because they were unresponsive in the presence of cycloalkanes.

4.2. Principal component screening

A total of 24 compounds comprising the prediction frame were screened, consisting of C7-C18 *iso*-alkanes, C8-C17 monocycloalkanes, and C11-C14 dicycloalkanes, with predicted volume swell values and cumulative importances for compounds displayed in the [Supplementary Material](#). Of the 24 compounds screened, only four -*cis*-1,2-dimethylcyclooctane, pentylcyclohexane, hexylcyclohexane, and *sec*-butyldecalin- met the 90% feature importance threshold. No *iso*-alkanes met the screening criteria, likely because farnesane was the only *iso*-alkane used to train the model. Lighter *iso*-alkanes generally fell out at PC21, while heavier *iso*-alkanes fell out at PC22. Both PCs are associated with cycloalkane and aromatic ring descriptors, indicating that training the model on a diverse set of compound groups inhibits predictions for some compound groups because it necessitates the creation of irrelevant features. Many mono- and dicycloalkanes, such as decyl- and undecylcyclohexane, were also outside the range of PC22 because of their high molar volumes.

4.3. HPF optimization (value and performance)

Fig. 6 shows the SE vs. ED Pareto front consisting of 7196 solutions representing optimized blends of 10 compounds. The red hexagons represent conventional jet fuels, which serve as the origin for the plot. Symbols with colored outlines represent compounds found in conventional jet fuel, with the gray fill indicating compounds that were used for optimization. Compounds with the blue fill were not used because volume swell data was not available or because they are not desirable in the case of aromatics. The blue line represents the ‘best-case’ conventional fuels, which are fuels from the Petroleum Quality Information System [21] with the highest energy values. The dark blue shaded region to the right of the “best-case” conventional fuels line has been deemed the HPF region. This region is bound by the straight blue lines which represent density limits. Any fuel that falls within the HPF region and meets operability limits is considered a HPF.

Median SE and ED 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 an average conventional jet fuel [22]. The Pareto front is fairly

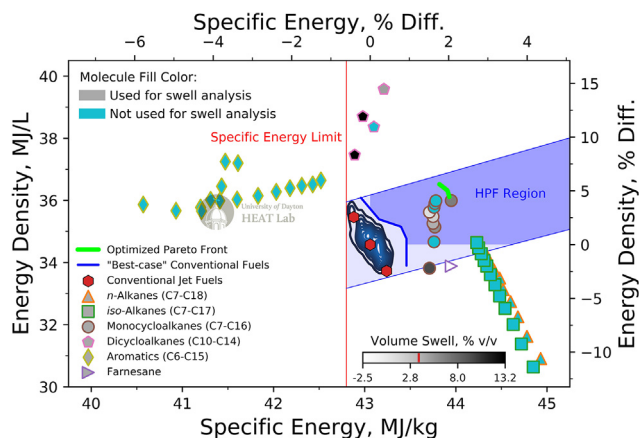


Fig. 6. SE plotted against ED with the HPF Pareto front representing blends of *iso*- and cycloalkanes meeting nitrile rubber volume swell requirements in addition to other operability limits.

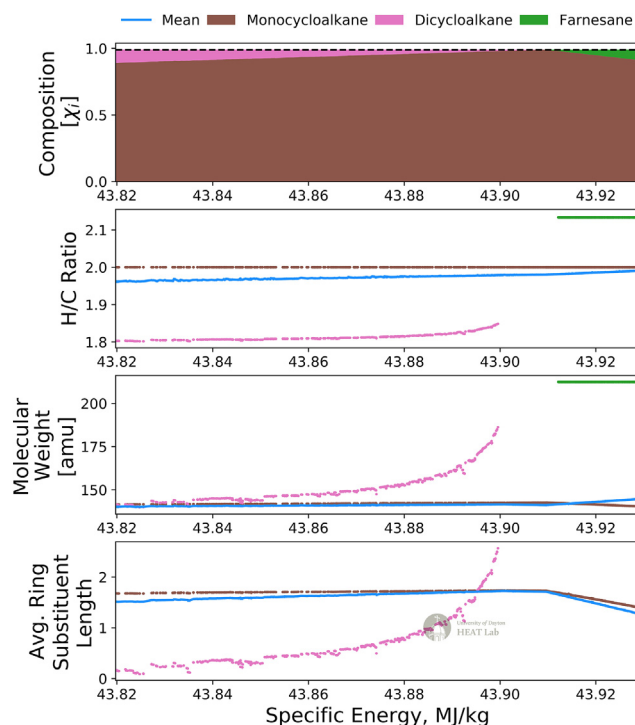


Fig. 7. Composition and compound structure of solutions across the HPF Pareto front.

constrained relative to previous optimization efforts which spanned the majority of the density region. The Pareto front is limited on the right because it cannot achieve a higher SE than the set of compounds used for optimization. Specifically, the highest SE 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 Fig. 6 because reproducibility uncertainty is incorporated into the optimization constraints to provide a factor of safety.

4.4. HPF optimization (composition and compound structure)

Composition and compound structure for solutions across the Pareto front can be seen in Fig. 7, with blue lines representing mean blend values. Solutions consisted primarily of monocycloalkanes because of their high SE, advantageous volume swell, and position within the density range. Monocycloalkanes were 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. If more *iso*-alkanes were used for optimization, such as those represented by squares in Fig. 6, it is likely that they would be used to increase the SE of solutions. 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.

The H/C ratio and molecular weight of dicycloalkanes increased as higher SE solutions were attained, indicating higher concentrations of *sec*-butyldecalin in favor of unsubstituted decalins. The decrease in substituent length of monocycloalkanes starting at 43.91 MJ/kg can be attributed to increasing concentrations of light monocycloalkanes as the optimization algorithm tried to pull the Pareto front toward lower ED solutions.

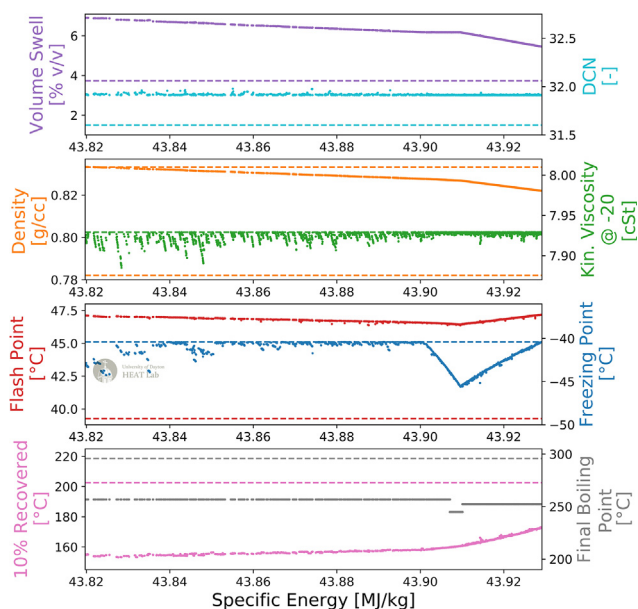


Fig. 8. Operability and safety properties of solutions across the HPF Pareto front.

4.5. HPF optimization (operability and safety)

Operability and safety properties of solutions across the Pareto front can be seen in Fig. 8, 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. It is likely that if more *iso*-alkanes were used for optimization, volume swell would serve as a limiting factor as higher SE solutions were achieved. The high volume swell of solutions attests to the favorable volume swell characteristics of cycloalkanes. DCN remained consistent across the Pareto front, with a standard deviation of 0.008. Compounds 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 additional dicycloalkanes. It scaled with volume swell, decreasing linearly as dicycloalkanes were removed and as farnesane was added. Viscosity varied little with a standard deviation of 0.005 cSt. Viscosity remained close to its upper limit, indicating that it was a difficult constraint to achieve. This is likely because of the high viscosity of *cis*-1,2-dimethylcyclooctane, which was favored across solutions. Viscosity fluctuation increased in magnitude as dicycloalkanes were added, likely because of increased sensitivity to composition as high viscosity compounds were added.

Flash point remained well above its limit of 38 °C. Volume swell and flash point are in competition with one another because volume swell has an inverse relationship with molar volume while flash point has a direct relationship with molar volume. If lighter *iso*-alkanes were used to increase SE, it is likely that the flash point of solutions would decrease. 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. Outside this range, freezing point served as a limiting constraint for the optimization.

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 compound in the solution. Compounds 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 *iso*- and cycloalkanes.

5. Conclusion

A framework has been developed to predict volume swell of non-metallic materials submerged in neat compounds. Subsequent optimization was performed to identify blends of compounds that maximize energy while remaining within 'drop-in' limits and meeting novel swell requirements. Volume swell predictions for 3 materials -nitrile rubber, extracted nitrile rubber, and polythioether- had sufficient accuracies for first-order optimization. Optimized blends achieved an average nitrile rubber volume swell of 6.2% v/v, well within the 3.7–17.4% v/v range of conventional jet fuels. Additionally, median SE and ED gains of 1.9% and 5.1% were reached, which can increase the payload and range of flights in addition to reducing the volume of fuel required.

This study indicates that cycloalkanes are a suitable replacement for aromatics considering volume swell requirements. The emissions reduction from replacing aromatics with cycloalkanes would be significant: cycloalkanes produce 88% less soot on average compared to aromatics [23]. It is estimated that direct radiative forcing from aviation-related soot emissions is 9.5 mW/m² [24], approximately 12% of the total RF associated with aviation [25]. It follows that the replacement of aromatics with cycloalkanes could reduce RF associated with aviation by roughly 10.6%.

Taking additional optical dilatometry measurements to increase the isomeric variance of the compounds used to train the neural network can improve model accuracy and expand the range of predictions that can be made, in addition to validating Eq. (1) used for optimization. In general, specific neural network models for each compound group and material are preferable because they eliminate unnecessary features such as ring descriptors for *iso*-alkanes and material descriptors, the latter of which accounted for 10 of 27 features used for model training in this work.

CRediT authorship contribution statement

Shane Kosir: Conceptualization, Methodology, Software, Validation, Formal analysis, Data curation, Writing - original draft, Writing - review & editing, Visualization, Funding acquisition. **Joshua Heyne:** Conceptualization, Methodology, Resources, Writing - review & editing, Supervision, Funding acquisition. **John Graham:** Conceptualization, Methodology, Resources, Writing - review & editing.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2020.117832>.

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