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Research Article

Machine Learning-Based Prediction of Sustainable Aviation Fuel Yield using Literature-Derived Hydroprocessing Data

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ABSTRACT

The increasing demand for sustainable aviation fuel (SAF) has encouraged the development of efficient predictive approaches for optimizing jet fuel production from renewable feedstocks. Conventional experimental optimization methods are often time-consuming and expensive because hydroprocessing performance is strongly influenced by feedstock characteristics, catalyst composition, and operating conditions. In this study, machine learning (ML) techniques were applied to predict jet fuel yield using a dataset compiled from approximately 50 published scientific articles. The dataset consisted of 101 experimental observations involving different feedstock groups, catalyst metal groups, catalyst supports, catalyst loading, free fatty acid (FFA) content, temperature, pressure, and weight hourly space velocity (WHSV). The ML workflow was developed using Orange Data Mining software and included data preprocessing, feature selection, imputation, model training, and performance evaluation. Four regression algorithms, namely Random Forest, Linear Regression, Neural Network, and Gradient Boosting, were evaluated using 10-fold cross-validation. The Gradient Boosting model achieved the best predictive performance with an RMSE of 7.172, MAE of 5.314, MAPE of 10.026%, and R2 value of 0.286 during cross-validation. Feature ranking analysis indicated that catalyst support type, feedstock group, catalyst metal group, and FFA content were among the most influential variables affecting jet fuel yield.

1. INTRODUCTION

The aviation industry is one of the largest contributors to greenhouse gas emissions among transportation sectors. The increasing global demand for air transportation has intensified the need for alternative fuels capable of reducing carbon emissions while maintaining compatibility with existing aircraft infrastructure. Sustainable aviation fuel (SAF) has emerged as a promising solution because it can significantly reduce lifecycle greenhouse gas emissions compared with conventional fossil-based jet fuel. Hydroprocessed esters and fatty acids (HEFA) pathways are among the most mature technologies for SAF production due to their compatibility with current aviation systems and their ability to produce high-quality jet fuel fractions.

The production of jet fuel from renewable feedstocks is influenced by many factors, including feedstock composition, catalyst type, catalyst support, operating temperature, pressure, and residence time. Experimental optimization of these variables requires extensive laboratory work, large operational costs, and long experimental durations. Consequently, computational methods capable of predicting product yield using historical data have become increasingly important.

Machine learning (ML) has recently gained attention in chemical engineering and biofuel research because of its ability to identify nonlinear relationships between process variables and product performance. ML models have been successfully applied in biomass conversion, catalyst optimization, and fuel property prediction. Compared with

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conventional statistical methods, ML algorithms can process complex datasets and provide better predictive accuracy for multifactor systems.

In recent years, the integration of machine learning with sustainable aviation fuel research has shown considerable potential for accelerating process optimization and reducing experimental efforts. Previous studies have highlighted the importance of artificial intelligence and data-driven approaches for predicting fuel properties, catalyst performance, and biofuel production efficiency [1]. In addition, hydroprocessing-based SAF production has been widely investigated due to its high compatibility with aviation fuel standards and its ability to utilize renewable lipid feedstocks [2].

This study aims to develop a machine learning model for predicting jet fuel yield using experimental data collected from approximately 50 scientific publications. The research employed Orange Data Mining software to construct a regression-based workflow involving feature selection, preprocessing, model comparison, and prediction analysis. Four ML algorithms, including Random Forest, Linear Regression, Neural Network, and Gradient Boosting, were evaluated to identify the most suitable model for predicting SAF yield. The developed model was subsequently applied to new experimental data obtained from thesis research in order to evaluate its predictive capability.

2. METHOD

2.1 Dataset Collection

The dataset used in this study was compiled from approximately 50 published scientific papers related to sustainable aviation fuel and hydroprocessing-based bio-jet fuel production [10-59]. A total of 101 experimental observations were collected and organized into a structured database. The variables included feedstock group, free fatty acid (FFA) content (%), catalyst metal group, catalyst loading (%), catalyst support group, reaction temperature (T), reaction pressure (P), weight hourly space velocity (WHSV), and jet fuel yield (%) as the target variable. The feedstocks included palm-based oils, vegetable oils, waste oils, algae-based oils, and pure compounds. Catalyst systems included noble metals, transition metals, and bimetallic catalysts supported on oxide, zeolite, mesoporous, carbonaceous, and molecular sieve materials.

Table 1.
Example of dataset used for machine learning model development

No	Feedstock-Group	FFA (%)	Metal-Group	Loading (%)		Support-Group	T (C)	P (bar)	WHSV	Yield Jet
1	Palm-based	5	Noble Metal	5	....	Carbonaceous	420	34	16	58,29
2	Palm-based	5	Noble Metal	5	....	Carbonaceous	400	34	4,19	59
3	Pure Compound	2	Bimetallic	5	....	Oxide	360	30	2	60
4	Palm-based	90	Bimetallic	10	....	Mesoporous	330	30	1	83
5	Palm-based	3	Noble Metal	8	....	Carbonaceous	400	1	1	73

Only representative data samples are presented in this paper, while the complete dataset consisted of 101 experimental observations collected from approximately 50 scientific publications [10-59].

2.2 Machine Learning Workflow

The machine learning workflow was developed using Orange Data Mining software. The workflow consisted of several stages, including data import, feature selection, preprocessing, model development, model evaluation, and prediction. The workflow structure included file import and data loading, data preprocessing using Edit Domain and Impute widgets, feature ranking and selection using ReliefF analysis, model training using multiple regression algorithms, model evaluation through Test and Score, and prediction of new experimental data. The workflow enabled systematic comparison of multiple regression algorithms using the same dataset and preprocessing strategy.

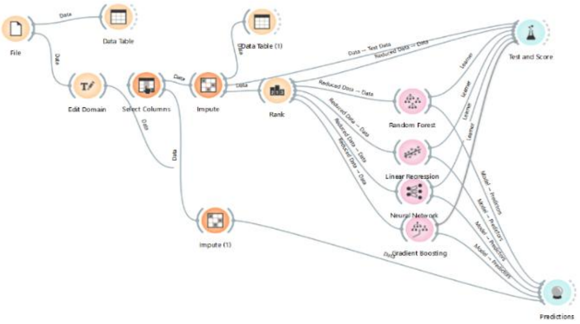


Figure 1. Orange Data Mining workflow used for jet fuel yield prediction.[9]

2.3 Feature Selection

Feature importance analysis was performed using the ReliefF algorithm in Orange. The ranking results showed that several variables had stronger influence on jet fuel yield prediction. The most influential variables were support group, feedstock group, catalyst metal group, FFA content, and catalyst loading. The WHSV parameter showed relatively low importance compared with other process variables.

2.4 Machine Learning Models

Four regression algorithms were evaluated in this study. Random Forest is an ensemble learning algorithm based on multiple decision trees that combines predictions from individual trees to improve predictive stability and reduce overfitting [10]. The algorithm works by generating multiple trees using randomly selected subsets of data and predictor variables, and the final prediction is obtained through averaging the outputs of all trees.

This approach enables Random Forest to effectively handle nonlinear relationships and heterogeneous datasets containing both numerical and categorical variables [11]. In the context of sustainable aviation fuel (SAF) production, Random Forest is suitable because hydroprocessing performance is influenced by complex interactions among feedstock composition, catalyst properties, operating temperature, pressure, free fatty acid (FFA) content, and weight hourly space velocity (WHSV). The algorithm is capable of identifying hidden patterns within literature-derived hydroprocessing datasets and has been widely applied in chemical engineering studies involving multifactor systems and process optimization [12].

Linear Regression was used as a baseline model to evaluate the linear relationship between process variables and jet fuel yield [13]. The model estimates the target variable by fitting a linear equation to the observed data, assuming that the dependent variable changes proportionally with the independent variables. Although hydroprocessing reactions involve highly nonlinear mechanisms, Linear Regression remains useful because of its simplicity, interpretability, and low computational requirements. In this study, the model was applied to provide a reference point for comparing the predictive capability of more advanced machine learning algorithms. The use of Linear Regression also enabled evaluation of whether process variables such as catalyst loading, reaction temperature, and pressure exhibit partially linear relationships with sustainable aviation fuel yield [14].

The Neural Network model was implemented to capture nonlinear relationships among process variables using interconnected computational nodes organized into input, hidden, and output layers [15]. Neural Networks are inspired by the structure of the human brain and are capable of learning complex patterns from large datasets through iterative training processes.

In hydroprocessing-based SAF production, numerous variables simultaneously affect catalytic cracking, deoxygenation, and hydroisomerization reactions, resulting in highly nonlinear process behavior. Neural Networks are theoretically capable of modeling these interactions more effectively than conventional statistical approaches because they can learn hidden relationships without predefined mathematical equations [16]. In this study, the Neural Network algorithm was evaluated to determine its ability to predict jet fuel yield using literature-derived experimental data involving various feedstocks, catalyst systems, and operating conditions.

Gradient Boosting is an ensemble learning technique that sequentially improves model performance by minimizing prediction error using multiple weak learners, commonly decision trees [17]. Unlike Random Forest, which constructs trees independently, Gradient Boosting develops trees sequentially, where each new tree focuses on correcting the errors produced by the previous model.

This iterative learning mechanism enables the algorithm to achieve high predictive accuracy and effectively model nonlinear interactions among variables. In sustainable aviation fuel research, hydroprocessing performance depends on complicated relationships between catalyst support, feedstock type, reaction conditions, and catalyst composition.

Gradient Boosting is highly suitable for this application because it can capture subtle interactions within heterogeneous datasets compiled from multiple literature sources. The algorithm has been widely recognized for its strong predictive performance in chemical engineering and process optimization studies involving complex experimental data [18].

2.5 Model Evaluation

Model performance was evaluated using 10-fold cross-validation. The evaluation metrics included Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), and Coefficient of Determination (R2). The best-performing model was selected based on the lowest prediction error and highest R2 value. The interpretation of MAPE values followed the prediction accuracy criteria reported by Maysoon (2023) and Utami (2019), as presented in Table 2.

Table 2.
MAPE interpretation criteria

MAPE Value	Interpretation
< 10%	Very good prediction capability (highly accurate)
10%–20%	Good prediction capability (accurate)
20%–50%	Reasonable prediction capability (moderately accurate)
> 50%	Poor prediction capability (inaccurate)

Based on this classification, the Random Forest and Gradient Boosting models in this study can be categorized as having good predictive capability because both models produced MAPE values close to 10%. Meanwhile, the Neural Network model demonstrated poor predictive performance due to its high MAPE value exceeding 50%.

2.6 Prediction of Experimental Data

After model training and validation, the developed models were used to predict jet fuel yield for new experimental data. The thesis dataset consisted of palm-based feedstock processed using noble metal catalysts supported on zeolite under varying temperatures.

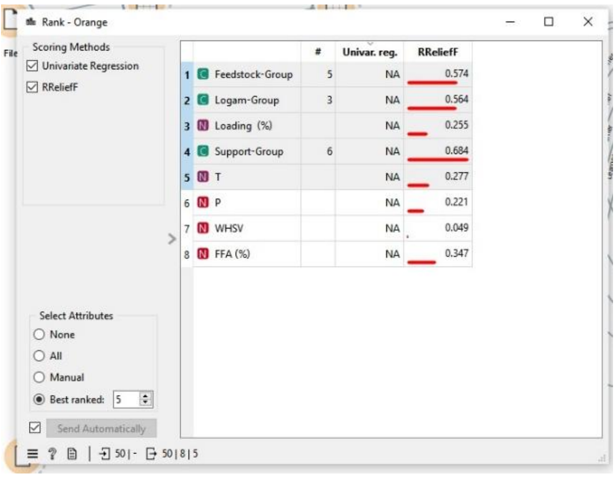
3. RESULT AND DISCUSSION

3.1 Machine Learning Workflow

The Orange workflow successfully integrated data preprocessing, feature ranking, model training, and prediction into a single analytical framework. The workflow simplified the evaluation of multiple regression algorithms while ensuring consistent preprocessing of the experimental dataset. The use of imputation widgets allowed missing values to be handled effectively, reducing the impact of incomplete experimental information collected from literature sources.

3.2 Feature Importance Analysis

Feature ranking results indicated that catalyst support group had the highest importance score among all variables. This finding suggests that support material strongly affects catalytic cracking, deoxygenation, and isomerization reactions during SAF production. Feedstock group and catalyst metal group also showed high influence on jet fuel yield prediction. This result is consistent with previous studies indicating that feedstock composition and catalyst characteristics strongly determine hydroprocessing efficiency and selectivity toward jet fuel fractions [2]. FFA content also contributed significantly to yield prediction because high FFA concentrations may influence deoxygenation pathways and catalyst stability. The relatively low importance of WHSV suggests that catalyst composition and reaction chemistry play more dominant roles than flow rate conditions in the compiled dataset.



☑ Univariate Regression
☑ RReliefF

		#	Univar. reg.	RReliefF
1	C Feedstock-Group	5	NA	0.574
2	C Logam-Group	3	NA	0.564
3	N Loading (%)		NA	0.255
4	C Support-Group	6	NA	0.684
5	N T		NA	0.277
6	N P		NA	0.221
7	N WHSV		NA	0.049
8	N FFA (%)		NA	0.347

○ None
○ All
○ Manual
● Best ranked: 5

☑ Send Automatically

Figure 2. Orange Data Mining feature importance (rank)

The feature importance analysis using the RReliefF algorithm in Orange Data Mining revealed that several variables had significant influence on jet fuel yield prediction. Based on the ranking results, the support group showed the highest importance score (0.684), indicating that catalyst support material was the most influential variable affecting sustainable aviation fuel (SAF) yield. This result suggests that catalyst support plays a major role in determining catalytic activity, hydrocracking performance, deoxygenation efficiency, and product selectivity during the hydroprocessing process. Different support materials such as zeolites, oxides, mesoporous materials, and carbon-based supports can strongly influence pore structure, acidity, metal dispersion, and reaction pathways, ultimately affecting jet fuel production efficiency.

The feedstock group and metal group (catalyst metal group) also demonstrated relatively high importance scores of 0.574 and 0.564, respectively. These findings indicate that both feedstock characteristics and catalyst metal composition significantly affect hydroprocessing reactions and jet fuel yield. Different feedstocks contain varying fatty acid compositions, oxygen content, and impurity levels, which may influence cracking behavior and hydrodeoxygenation reactions. Similarly, catalyst metals such as Ni, Co, Mo, Pt, and Pd possess different catalytic activities and hydrogenation capabilities that affect the conversion of triglycerides and fatty acids into jet fuel range hydrocarbons.

The FFA (%) variable also showed considerable influence with an importance score of 0.347. This result indicates that free fatty acid content contributes to determining reaction performance and product distribution during hydroprocessing. High FFA content may alter deoxygenation pathways, affect catalyst stability, and influence coke formation, thereby impacting sustainable aviation fuel yield.

Catalyst loading (%) produced a moderate importance score of 0.255, suggesting that the amount of active metal deposited on the catalyst support contributes to reaction efficiency but is less dominant compared with catalyst support and feedstock type. Reaction pressure (P) also demonstrated moderate influence with a score of 0.221, indicating that hydrogen pressure still affects hydroprocessing performance, although its impact was lower than catalyst-related variables.

Among all evaluated variables, WHSV showed the lowest importance score (0.049). This finding suggests that flow rate conditions had relatively minor influence on jet fuel yield within the compiled literature-derived dataset. The result may indicate that catalyst properties and feedstock characteristics play more dominant roles than residence time effects under the investigated operating conditions.

Overall, the feature importance analysis demonstrates that catalyst characteristics and feedstock properties are the primary factors governing sustainable aviation fuel yield during hydroprocessing. These findings are consistent with previous studies reporting that catalyst support, catalyst metal composition, and feedstock composition strongly influence hydrodeoxygenation, hydrocracking, and hydroisomerization reactions in SAF production systems.

3.3 Model Performance Evaluation

The performance comparison of the four machine learning models is summarized in Table 3. Among all evaluated models, Gradient Boosting produced the best performance with the lowest RMSE, MAE, and MAPE values. The model also achieved the highest R2 value, indicating better predictive capability compared with other algorithms. The Neural Network model showed very poor performance with extremely high prediction error. This result may be caused by the relatively limited dataset size and the presence of heterogeneous categorical variables. The superior performance of Gradient Boosting can be attributed to its ability to handle nonlinear relationships and interactions among process variables.

Table 3.
Cross-validation performance of machine learning models

Model	MSE	RMSE	MAE	MAPE	R^2
Random Forest	58.048	7.619	5.477	10.306	0.194
Linear Regression	91.348	9.558	6.305	11.659	-0.269
Neural Network	1218.000	34.901	34.069	63.828	-15.00
Gradient Boosting	51.434	7.172	5.314	10.026	0.286

The comparative evaluation of machine learning models provides important insight into the applicability of predictive analytics for sustainable aviation fuel production. RMSE and MAPE are widely used metrics to evaluate prediction accuracy and model robustness.

Gradient Boosting demonstrated the best overall predictive capability among the evaluated models. The low RMSE and MAPE values indicate that the model was able to capture nonlinear relationships between catalyst properties, feedstock characteristics, and operating conditions. Random Forest also showed relatively strong predictive performance due to its ensemble-learning mechanism. However, the model produced slightly higher prediction error compared with Gradient Boosting.

Linear Regression provided acceptable prediction results but was limited in capturing complex nonlinear interactions among variables. This limitation is expected because hydroprocessing reactions involve highly nonlinear chemical phenomena.

The Neural Network model produced the poorest predictive performance in this study. The relatively small dataset size and heterogeneous categorical variables may have reduced the capability of the neural network to generalize accurately.

However, although Gradient Boosting demonstrated the best predictive performance among the evaluated models, the relatively low coefficient of determination ($R^2 = 0.286$) indicates that a substantial proportion of the variability in SAF yield remains unexplained. This result suggests that the complexity of SAF production may not be fully represented by the variables included in the current dataset. Consequently, the model should be interpreted as a tool for identifying general trends and relationships among process variables rather than for highly accurate yield prediction. Nevertheless, its ability to capture meaningful patterns provides valuable insights for preliminary process evaluation and decision-making.

The integration of visualization techniques such as bar charts also can improve interpretation of machine learning performance and facilitate comparison between algorithms.

3.4 Prediction Analysis on Experimental Data

The trained machine learning models were subsequently applied to experimental data involving PFAD feedstock processed over cobalt- and nickel-supported HZSM-12 catalysts under different reaction temperatures. The experimental data were obtained from a previous study reported by Alel (2019)[69]. The experimental data reported jet fuel yields ranging from 44% to 55.5% using Ni- and Co-based noble metal catalysts. The prediction results generated by the machine learning models are presented in Table 4.

Table 4.
Prediction results for thesis experimental data

T(°C)	Exp Yield (%)	Random Forest	Linear Regression	Neural Network	Gradient Boosting
350	44–55.5	54.0	50.60	16.09	57.86
375	44–55.5	55.9	53.44	15.74	58.02
400	44–55.5	69.22	56.27	16.30	71.07

The prediction results demonstrated that Random Forest and Linear Regression produced predictions closer to the experimentally observed yield range compared with Gradient Boosting and Neural Network models. At reaction temperatures of 350°C and 375°C, Random Forest predictions remained relatively close to the upper experimental yield range. In contrast, the Neural Network model consistently underpredicted the jet fuel yield, with predicted values only around 16%, significantly lower than the actual experimental observations.

Although Gradient Boosting achieved the best cross-validation performance during model evaluation, its predictions at 400°C substantially overestimated the jet fuel yield. This behavior may indicate mild overfitting caused by the relatively limited size and heterogeneous nature of the literature-derived dataset. The discrepancy between training performance and external validation performance indicates that model generalization capability should be carefully evaluated using independent experimental data. This finding highlights the importance of external validation in machine learning studies involving chemical engineering datasets.

Overall, the prediction analysis confirmed that literature-based machine learning models can provide useful preliminary estimation of sustainable aviation fuel yield under new operating conditions. Such predictive capability can reduce experimental screening effort and support catalyst optimization during SAF development.

3.5 Implications for Sustainable Aviation Fuel Development

The integration of machine learning with SAF production research offers several important advantages, including faster prediction of process performance, reduced experimental cost and time, identification of influential process variables, improved catalyst and operating condition selection, and acceleration of SAF process optimization. The present study demonstrates that literature-based datasets can be effectively utilized for ML model development. This approach is particularly valuable for emerging SAF technologies where experimental data are scattered across many publications.

The findings also support previous studies reporting that machine learning can accelerate sustainable fuel research by enabling predictive process analysis and intelligent optimization strategies [1]. Despite promising results, several limitations remain.

Furthermore, the dataset used in this study was compiled from multiple independent studies that differed in experimental design, reactor configuration, feedstock characteristics, yield definitions, and analytical methods. Such data heterogeneity may introduce additional variability and uncertainty into the dataset, which may affect the reliability and generalizability of the predictive models. Therefore, the model results should be interpreted with consideration of the differences among the original data sources.

Nevertheless, the use of a diverse dataset enables the models to capture broader trends that may be representative of a wider range of SAF production conditions. Future studies should focus on data standardization, the inclusion of additional process variables, and the development of models based on larger and more homogeneous datasets to further improve predictive performance and robustness.

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4. CONCLUSIONS

This study successfully developed a machine learning-based approach for predicting sustainable aviation fuel yield using hydroprocessing data collected from approximately 50 scientific publications. The Orange Data Mining workflow enabled efficient preprocessing, feature ranking, model training, and prediction analysis. Four regression algorithms were evaluated, namely Random Forest, Linear Regression, Neural Network, and Gradient Boosting.

Among the evaluated models, Gradient Boosting showed the best predictive performance with RMSE of 7.172, MAE of 5.314, MAPE of 10.026%, and R2 value of 0.286 during cross-validation. Feature importance analysis revealed that catalyst support group, feedstock type, catalyst metal group, and FFA content were the most influential variables affecting jet fuel yield.

The developed models were successfully applied to predict yield for new experimental data, demonstrating the potential of machine learning for reducing experimental effort and accelerating SAF process optimization. Future work should focus on expanding the dataset, integrating additional physicochemical parameters, and applying more advanced machine learning techniques to improve prediction accuracy.

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