Project 033 Alternative Jet Fuels Test Database (AJFTD) Library (2022)

University of Illinois Urbana-Champaign

Project Lead Investigator

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- P.I.: Tonghun Lee, Professor
- FAA Award Number: 13-C-AJFE-UI-038
- Period of Performance: October 1, 2021 to September 30, 2022
- Tasks:
    1. Online database development with JETSCREEN, ALIGHT, NewJET, and domestic airport connection
    2. Machine-learning-based online analysis

Project Funding Level

FAA funding level: $150,000
Cost sharing: Software license support from Reaction Design (ANSYS)

Investigation Team

- Tonghun Lee (Professor, University of Illinois at Urbana-Champaign): overall research supervision
- Alex Solecki (Graduate Student, University of Illinois at Urbana-Champaign): database development
- Ji Hun Oh (Graduate Student, University of Illinois at Urbana-Champaign): machine-learning-based analysis

Project Overview

This study seeks to develop a comprehensive and foundational database of current and emerging alternative jet fuels by integrating relevant pre-existing jet fuel data into a common archive that can support scientific research, enhance operational safety, and provide guidelines for the design and certification of new jet fuels. In light of the September 2021 White House statement on advancing the future of sustainable aviation fuels (SAFs) in America, the database now has even greater potential for serving the national agenda. In previous years of this project, efforts focused on the integration and analysis of pre-existing jet fuel data from various government agencies and individual research groups. In 2020, we converted all the compiled data to a new nonstructured query language (NoSQL) format by using a JavaScript object notation (JSON) schema, thus allowing the data to be analyzed in a flexible manner by using various programming languages. To this end, we have launched the second generation of our online database, the National Alternative Jet Fuels Test Database (AJFTD), which uses the new nonrelational database structure. This version is equipped with interactive analysis functions for users, and flexible methods for plotting and downloading data. In the previous year, we extended this effort to incorporate advanced machine learning algorithms into the analysis process. Additionally, we have integrated our database with the database assembled by the European JETSCREEN program. In the future, data acquisition from domestic and international airports will help further develop the database and support its use as a repository for all SAF-related property and test data.

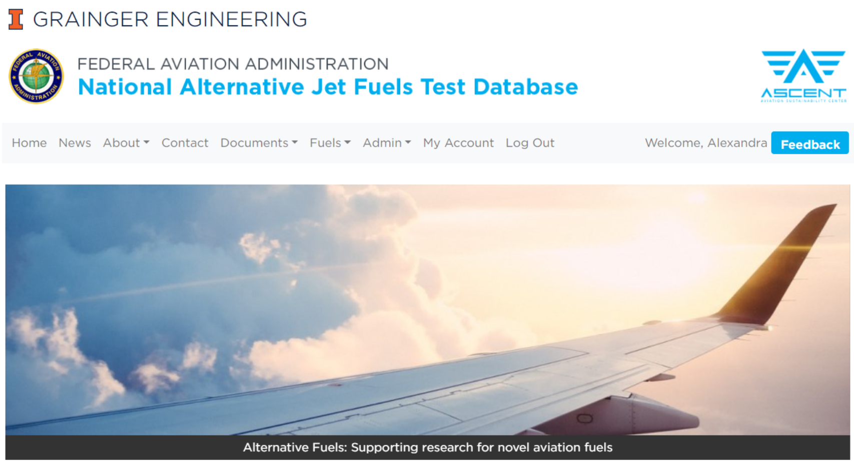

Figure 1. Alternative Jet Fuels Test Database homepage.

We hope that the database will, one day, serve not only as a comprehensive and centralized knowledgebase used by the jet fuel research community, but also as a resource to enhance global operation efficiency and safety. Future efforts will include linking real-time fuel usage and certification data from domestic and international airports. Connecting our database with ongoing European projects, such as ALIGHT and NewJET, will help create avenues for future database development in this area. Given the prolific diversification of new alternative jet fuels expected in the near future, the ability to track critical fuel properties and test data from both research and operation perspectives will be highly valuable for the future of commercial aviation. Furthermore, increasing the breadth of data categories available on the database, from fuel data to global usage trends, will make the database relevant to a greater audience. We hope that ongoing website development and an improved user interface will also allow the general public to engage with high-level information regarding SAFs, thereby increasing the general public's knowledge and awareness of SAFs, and further supporting the national visibility of sustainable aviation.

Task 1 - Database Development: ALIGHT, NewJET, and Domestic Airport Connection

University of Illinois at Urbana-Champaign

Objectives

The main objective of this task is to upgrade and debug the generation II online AJFTD functions and link the database to the European ALIGHT and NewJET programs. The generation II database was designed by using a new architecture based on a NoSQL data format that allows for flexible analysis and scaling. This format can accommodate various data types that can be easily accessed by any common programming language, and basic analysis functions have been built directly into the web interface. Additionally, substantial effort has been made in the past year to improve the data organization and retrieval process for both website administrators and standard users. Ensuring that all users can efficiently locate and collect all relevant data samples for their purposes is the main objective for future website adjustments and improvements. The main Task 1 objectives are as follows:

- Detail data type, frequency, and sharing methods with the ALIGHT program led by Copenhagen Airport and the NewJET program led by the University of Birmingham
- Establish methods for acquiring real-time airport fuels data from domestic U.S. airports, beginning with Chicago O'Hare International Airport

Research Approach

Generation II Database Debugging and Upgrade

The current generation II version of the web interface for the AJFTD maintains most of the functional features present in the originally developed database. Much like generation I, generation II is an HTML-oriented program built on a layer of metadata, which supports search functions for users. The tree structure applied to organize the data folders in the first database has been retained in the second version, thereby allowing users to access the data in a similar manner. The main difference is that an additional inner core houses the JSON files, where the test data reside. Currently, the database has grown to house more than 25,000 separate fuel records.

The catalog of data currently available in the database is assembled primarily from four separate sources. The fuels with POSF (Air Force Research Laboratory fuel database code) number designations were added from the internal database maintained by the Air Force Research Laboratory at the Wright Patterson Air Force Base. The second dataset was obtained from the Petroleum Quality Information System (PQIS) reports of the Naval Air Systems Command and corresponds to a compilation of fuel data geared primarily toward government use. The third set was provided by Metron Aviation, which compiled fuel properties from samples collected at airports through a previous ASCENT project. The dataset resulting from this study has proven valuable by showing the landscape of fuels currently used in commercial aviation and will guide our future efforts focused on capturing this type of data in real time. The final dataset was obtained from the National Jet Fuel Combustion Program within ASCENT.

After the launch of the generation II database, substantial changes have been made to fix bugs and upgrade various aspects of the database. Some of the key changes to the database are summarized below.

- Efforts have been made to convert the JSON format on the database to a CSV format for select files to enable machine-learning-based analysis, which will be addressed further in Task 2. The actual files that are stored will use the NoSQL JSON format, which is conducive to maintaining a flexible database. However, certain parts of the data that are to be analyzed using machine learning will need to be converted to CSV format, for which multiple Python-based machine learning scripts are available. In the future, a process may be necessary to automate this conversion in real time.

- Online viewing of 2D gas chromatography (GCxGC) data has been made available to users. The scripts that process data uploads have been revised to properly process the section containing GCxGC data and now present this information on the web portal. This is an important development, because it is the first of many upcoming improvements to the user interface that will allow users to engage with data on the website itself in a comprehensive and high-level fashion before downloading and processing raw files.

- The "Documents" categories have been updated to reflect a wider range of document categories (now available under "Documents" → "Browse by Category") including ASCENT reports for relevant alternative jet fuel projects and recent literature relating alternative jet fuels to flight and laboratory tests on emissions, contrails, etc.

- With an emphasis this year on the optimization of the data retrieval process, the acquisition of firsthand user feedback was a priority. A feedback portal has been added and is present on every page on the AJFTD to provide users with a quick and optionally anonymous method for reporting technical issues, usage concerns, questions, or all other feedback regarding the usage or content of the database. This option is presented in addition to existing contact information supplied under the "Contact" and "About" → "Directory" tabs.

- In prior website versions, the differences between the "Fuels" and "Documents" tabs were ambiguous, and the information was searchable under either or both tabs. To clarify the purposes of these two pages, an "About" page has been added to the "Documents" drop-down menu detailing the searchable results. Additionally, the "Fuels" page has been converted to a "Fuels" drop-down menu with a similar "About" page detailing the contents of the "Search Fuels" page, and how to navigate this page by using available filters and keywords.

- Similarly to the above point, various small changes and clarifications have been made to other drop-down categories such as changing "Categories" under the "Documents" drop-down to "Browse by Category," and inserting scroll-over buttons on pages such as "Search Fuels" for expanding upon the functionalities and intended uses of various interface features.

- Fuel data are organized and searchable under the "Fuels" tab according to various filter categories and keywords. However, many of these keywords and filters previously yielded either incomplete lists of results or results that were erroneously tagged or keyed. The issue was found to arise from several thousand JSON files that were unlabeled or erroneously labeled in various metadata categories (e.g., "fuel type" or "origin"). Python scripts have been written to comb through all database JSON files (>25,000) and retag them with the proper metadata categories. Fuel records for blends of multiple fuel types have been retagged with each blend component separated by a forward slash. In all cases, when a blend contains at least one conventional and at least one alternative fuel, the alternative fuel is listed first. If the blend comprises two alternative fuels, they are ordered alphabetically. If the blend contains only conventional fuels, the fuels are ordered alphabetically. This process was undertaken to eliminate ambiguity regarding the contents of the previously implemented "Blend" fuel type, to assist in efficient record retrieval. All retagged files have been reuploaded and are now searchable on the website.

- As displayed in Figure 2, the "Search Fuels" page now includes new filters for searching by fuel records containing data under certain compositions and property data categories (for searching for all results containing, for example, GCxGC data and/or flash point values). This functionality was inspired by increasing use of the database for generating datasets for training and testing models that map composition to properties; building such models would require quick filtering of all fuel records containing relevant data.

- An additional metadata category, "Fuel Class," has been created to support future development of a tool for quickly comparing a given fuel sample to all other fuel samples in a given category. Such a category may be an existing metadata category, such as "Fuel Type" or "Origin," or the new category "Fuel Class." This category aims to organize all fuel samples by more qualitative descriptions, sorting fuels into five main categories: Alternative Fuels, Blends, Conventional Fuels, Engineered Fuels, or Sustainable Aviation Fuels. Tagging fuels with these colloquial descriptions is intended to assist in higher-level engagement with fuel comparisons and data that are not restricted to a single fuel type; users may want to see how their fuel record compares with those of all previously approved SAFs, for example. This mass-comparison feature has not yet been fully developed; however, the "Fuel Class" metadata category is a preemptive development for supporting such a feature on a large scale and making the data on the website more accessible to a wider variety of users with various degrees of domain knowledge. We note that the "Sustainable Aviation Fuel" fuel class category is likely to be converted to "ASTM Approved Blendstocks" or some equivalent, because of the ambiguity surrounding the term "Sustainable Aviation Fuel" in the jet fuel market. A "Fuel Class" page will also be included under the "Fuels" drop-down menu; similarly to the "Fuel Type" page, it will clarify the distinctions made by website administrators.

- Website compare features have been updated to include the ability to compare multiple new composition categories including GCxGC data for various fuels (Figure 3). A 100% bar chart breaking down chemical family representation in the fuel sample is now displayed below the detailed composition bar chart, which separates a sample by chemical family and carbon number. This functionality is included for enhancing quick comparison between fuel samples by category as well as carbon number distribution. These bar charts also retain functionalities, such as the zoom, scroll-over detail, and on/off toggle, present on the complete composition bar chart. These comparisons can be exported similarly to other comparison results.

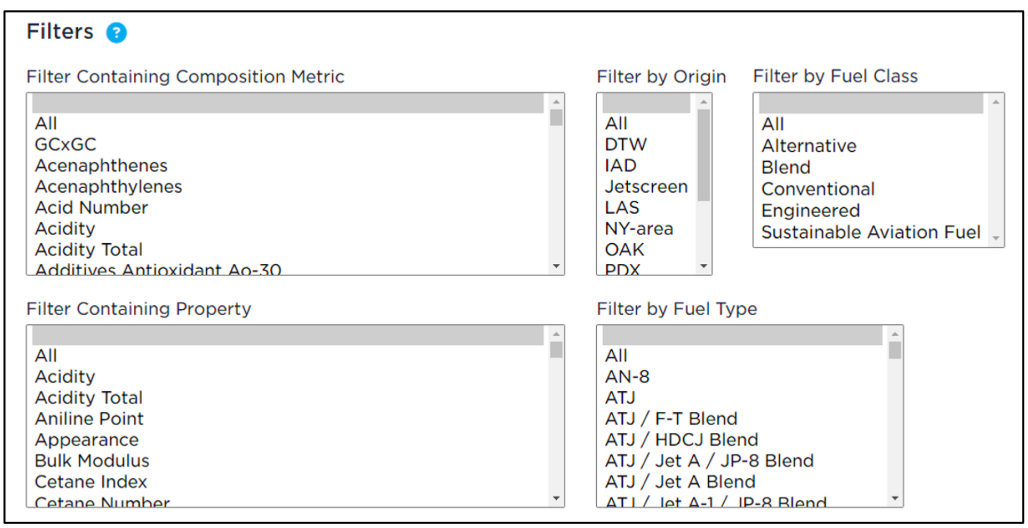

Figure 2. Updated fuel search bar filters and cleaned data sub-categories.

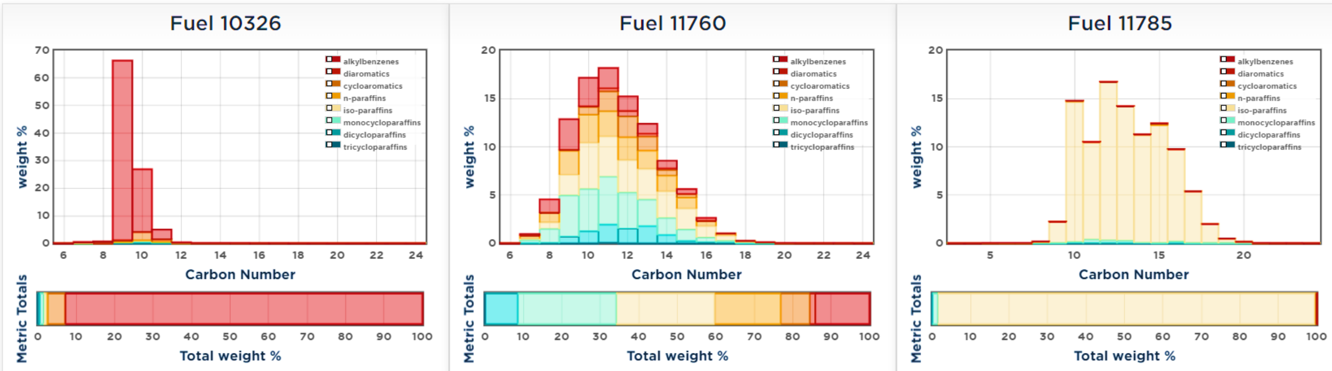

Figure 3. "Compare" functionality for GCxGC compositional data for various fuel samples.

Integration of the Database with JETSCREEN, ALIGHT, and NewJET

In 2020, we completed the integration of our database with the European JETSCREEN program. The JETSCREEN program was initiated (a) to provide fuel producers, air framers, and aero-engine and fuel system original equipment manufacturers with knowledge-based screening tools for fuels and (b) to produce a similar database that could be linked with ours. We first started discussing a potential merger with the JETSCREEN database in 2018, after which we started methodically synchronizing the data structure so that a merger would be possible. After extensive beta testing, the two databases were first linked in Spring of 2020. Data sharing between AJFTD and JETSCREEN ended in 2020 when the JETSCREEN project was completed and archived.

After the completion of JETSCREEN, AJFTD will continue to acquire new data through connection with the new European programs ALIGHT and NewJET. ALIGHT is a program aimed at assessing and improving the supply chain, integration, and use of SAFs and smart energy solutions through examining and optimizing operations at Copenhagen Airport. NewJET is a research program headed by the University of Birmingham, which is aimed at improving pathways for production of new SAFs. A similar data sharing structure is likely to be used to connect these programs with AJFTD, as was used with JETSCREEN; the process is outlined in Figure 4.

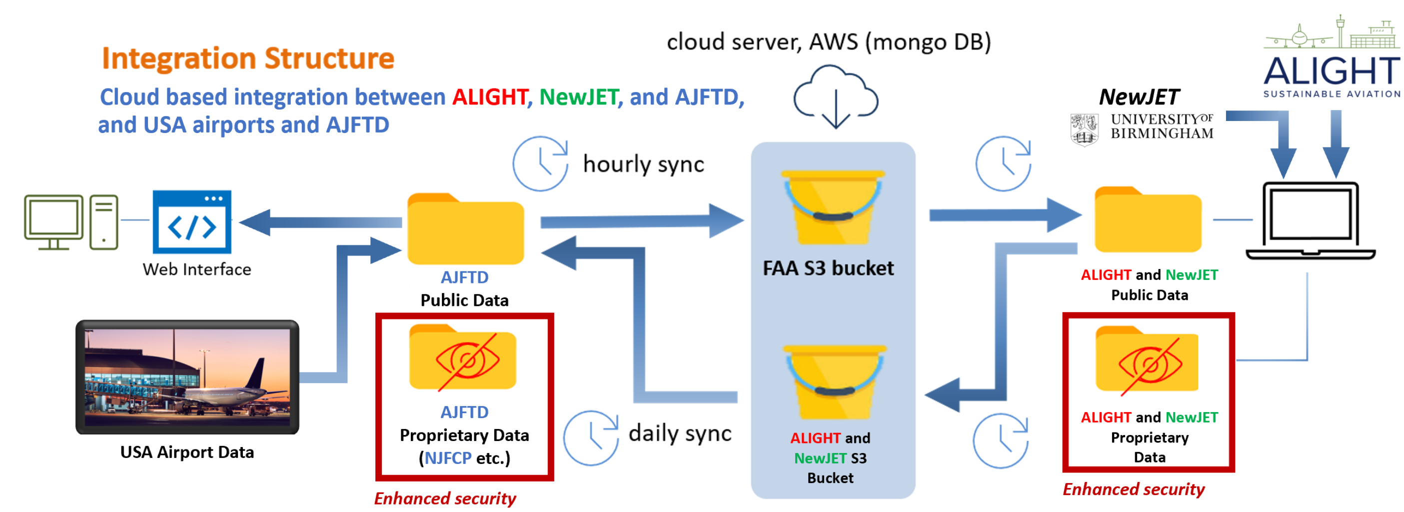

Figure 4. Plans for future data sharing with the European sustainable aviation programs ALIGHT and NewJET.

The JETSCREEN integration process helped streamline a data sharing method that ensures frequently updated and well-secured data flow between two projects; thus, this method of data sharing will probably also be used in future integration with the aforementioned ALIGHT and NewJET programs. Previously, the JETSCREEN and FAA databases were joined by a common cloud storage. Amazon Web Services was selected as the server to store the shared data, mainly because of its affiliation with the University of Illinois. S3 buckets (Amazon database structure) were created for both FAA and JETSCREEN to share their JSON files. Each could pull files from the other's folder, but read and write access was granted for only the owners of the bucket. The FAA data were shared to its S3 bucket via altjetfuels.illinois.edu. All public FAA data on the website had an option to be shared with JETSCREEN, and this option could be toggled by administrators. The website synchronized hourly with the bucket to upload newly shared data. No proprietary data were shared to the FAA S3 bucket. Any files uploaded to the FAA bucket could be viewed and downloaded by JETSCREEN. For downloading new JETSFCREEN data to the website, a script ran daily to verify JETSCREEN's S3 bucket for newly shared data. Any new files were then downloaded to our local database and could be accessed by users.

The completion of the JETSCREEN database integration process was a monumental first step in linking many other fuel databases worldwide. From this joint effort between FAA and JETSCREEN, we established a foundation for data sharing that can be used again with other programs, such as ALIGHT and NewJET. The ultimate goal of international database integration is to help monitor and evaluate fuels used in the international airspace and paint an accurate picture of how the fuel composition and usage trends are changing with time. As new fuels are integrated into the global supply chain, a means to keep track of their properties will become critical. Such an interconnected database will ensure provision of the most representative information needed for research and certification of new SAFs. The impacts of database integration are outlined in Figure 5.

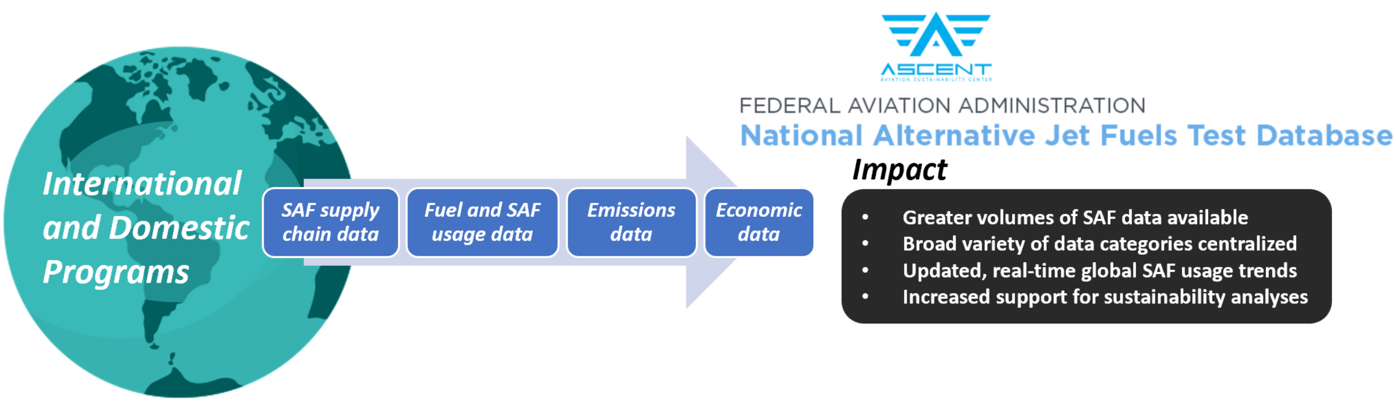

Figure 5. Plan to expand AJFTD's available data categories through data sharing with domestic airports, and the current international SAF projects ALIGHT and NewJET.

National motivation to achieve a more sustainable and emission-free aviation sector grew in the fall of 2021, with the announcement of the Sustainable Aviation Fuel Grand Challenge at a White House event. This initiative outlined a governmental approach for supporting SAF research, development, and implementation. As the topic gains national visibility, the platform for further development of the AJFTD is also growing.

In the past year, we have ramped up efforts to intercept fuel data from Chicago O'Hare International Airport. Efforts have included a variety of industry players including representatives from airlines, such as United Airlines, fuel testing facilities such as Nobil Petroleum Testing, and the FAA itself, among others. This effort requires extensive coordination at all levels of the aviation fuel industry, to acquire and formalize proper permissions for collection and publication of fuel data. Real-time acquisition of fuel data from the ground level on site at actual airports will be pivotal for converting the database from a static archive to a regularly updated monitoring tool for fuel trends in commercial aircraft. As alternative fuel deployment and incorporation into the supply chain accelerate, this data pipeline could serve as a crucial tool for measurement of the extent of the impact of blending on the compositions and properties of the fuel actively being used in commercial aircraft. The implications of such a tool are as diverse as supply chain analysis and the generation of fuel composition property datasets, as outlined in Figure 6.

This effort is expected to lay a foundation for achieving the sustainability targets set by both the U.S. (Sustainable Aviation Fuel Grand Challenge) and global community (Renewable Energy Directive II of the EU and the Paris agreement) by providing the data and analytic tools for sustainable pathways toward zero-emission airport operation through the integration of SAFs.

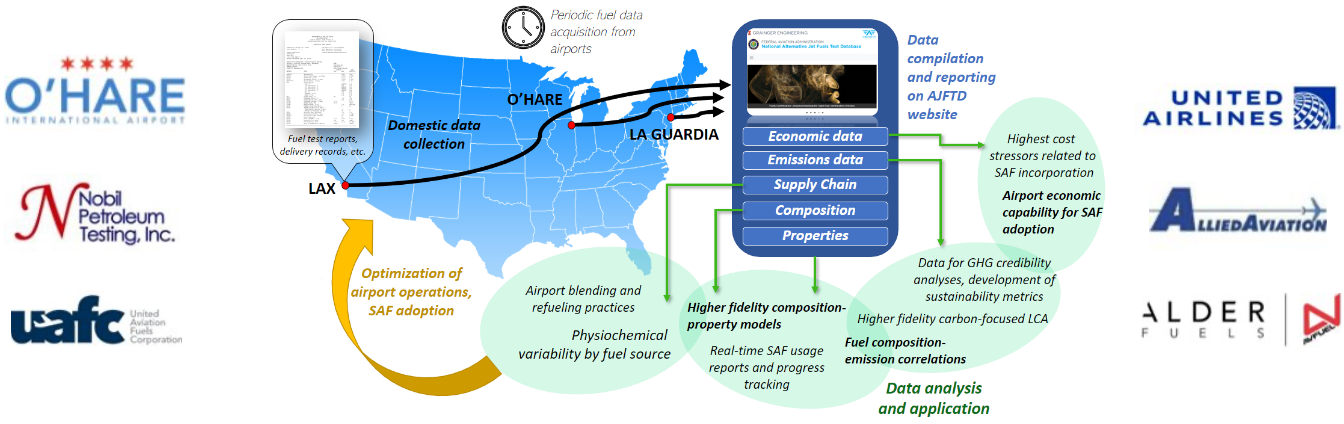

Figure 6. Domestic airport data collection scheme, publication, and potential effects.

Future efforts to broaden data sources for fuel data available on the website will include connection of our database with other ASCENT projects, including a newly piloted World Fuel Survey, which will largely replicate the global data collection process for the 2006 Coordinating Research Council's World Fuel Survey. This connection will provide a substantial source for the development of a dataset of recent, regionally representative conventional jet fuels' physical and chemical properties.

Milestones

3 months

- Debugging and optimization of the data structure in the generation II database
- Keyword fixes and resolution of search bar bugs
- Initial communication with Chicago O'Hare International Airport, United Airlines, Alder Fuels, and other industry partners

6 months

- Data cleaning commenced; all major JSON file bugs identified, and plan for scrubbing drafted
- New document sections live online
- User feedback tools built

9 months

- Python scrips completed for JSON editing; files cleaned and uploaded to website
- New search filters published to production site; troubleshooting complete
- Mission statement and formally documented plan for airport data collection finalized

12 months

- New interactive viewing features for comparing fuels finalized and published
- Communication with FAA contacts on next steps for airport data collection

Major Accomplishments

Initiation of Domestic Airport, ALIGHT, and NewJET Connections

Correspondence with relevant contacts for the aforementioned programs has been initiated and plans to proceed with international program integration are in place. These three connections will serve as new sources for acquiring greater amounts of fuel data, as well as the expansion of the data categories available on the database to categories such as usage and emissions data. Continued international collaboration will increase the long-term potential for support and data sharing with other international programs as they are formed. Connection with domestic airports will also support the long-term reliability of in-country data acquisition, if consistent avenues for data sharing are built and maintained, thus providing the database with the most up-to-date and relevant information available.

Modifications to the Generation II Online Database

The usability of the web interface is paramount to the purpose of the website. Data retrieval was addressed through the reconstruction of the search method on the backend site through frequent collaboration with the University of Illinois' web developer. The 25,000+ data files themselves were scanned, modified, and rewritten through various automated Python codes for eliminating redundancies, clarifying categories, and fixing tags and names in the fuel data and metadata categories. The modified files were then reuploaded to the website, and changes are reflected in updated search filter categories visible on the "Search Fuels" page. Search results now yield complete results and do not contain erroneously called fuel records.

Publication

Peer-reviewed journal publications

Oldani, A. L., Solecki, A. E., & Lee, T. (2022). Evaluation of physicochemical variability of sustainable aviation fuels. *Frontiers in Energy Research*, *10*, 1052267. doi: 10.3389/fenrg.2022.1052267

Outreach Efforts

The database has been made accessible through https://altjetfuels.illinois.edu/.

Awards

None.

Student Involvement

This project was conducted primarily by two graduate students (Alex Solecki and Ji Hun Oh).

Plans for Next Period

In the next period, the focus will be on ramping up progress in data collection from the aforementioned data sources: domestic airports, ALIGHT, and NewJET. In addition, pending the award of the project, the next World Fuel Survey will yield data in the coming years that will also be integrated into the database. Collaboration with all involved parties will ensure that the data are treated and represented properly online, and that all proprietary information is protected on both ends of the data sharing pipeline.

Additional efforts anticipated to improve the functional and aesthetic features of the database are summarized below.

- User interface and online analysis tools: The last year focused mainly on optimizing data retrieval and ensuring that the data currently available on the website are being called properly on the basis of relevant search filters and keywords. Moving forward, we will focus on user-driven interaction with the data after retrieval and will build a series of features to allow further first-level analysis of data. For example, a mass-compare function will be able to quickly build graphs and charts to compare the composition or properties of a single or group of fuel samples to all other samples in a relevant category, such as all samples of fuel type Jet A or all samples of fuel class SAF. These features will not only encourage use of the website but also make meaningful interaction with the data available to a wider audience.

- Domestic and international data collection: The focus of the next period will be to begin actual data transfer among Chicago O'Hare International Airport, ALIGHT, and NewJET. Because of the nature of fuel test data from on-site testing at domestic airports, some delays may occur in determining the proper contacts with authority to grant permissions to such data. This process remains underway, and we expect further progress in the coming months. Currently, no substantial obstacles prevent data sharing between Project 33 and the European ALIGHT and NewJET projects, and progress on these fronts is anticipated to be achieved soon in the next period.

Task 2 - Machine-Learning-Based Analysis

University of Illinois at Urbana-Champaign

Objectives

The main objective of this task was to develop advanced analysis methods based on machine learning algorithms for analysis of the data in the alternative jet fuel database. The effort is inspired by the notion that the intricate relations between properties of fuels and their chemical compositions are critical, but may be beyond the complexity that can be addressed in routine, classical, regression-based analysis. The effort becomes increasingly important as new analysis techniques, such as GCxGC, provide large amounts of data that are difficult to process with simple analytical algorithms. Machine learning can provide a means for the most advanced analysis to be applied to our current data, and this analysis should become even more powerful as the size and diversity of the data grow in the future. Previous work has verified the efficacy of artificial neural networks in modeling the complex and obscure correlations between jet fuels' chemical composition or structure and physicochemical properties. The next step of this task is to exploit neural networks and deep learning methods to address realistic challenges in SAF databases. Specifically, the major goals are as follows:

- Identify real-world challenges in the analyses of jet fuel, specifically SAFs and datasets
- Devise deep-learning-based strategies for addressing these challenges
- Perform composition–property modeling by using GCxGC and advanced machine learning techniques
- Specify the degree of uncertainty in such models and how to mitigate them

Research Approach

Data-driven Modeling and Uncertainty Quantification

In previous years, the machine learning applications focused on in this context were centered primarily around how to obtain a better predictive model for the properties of a given fuel, on the basis of its detailed chemical composition, typically obtained through a chemical separation method, such as GCxGC. However, higher predictive uncertainty was seen for alternative jet fuels than conventional fuels. To understand why, and to report on the required actions needed to decrease such uncertainty for future models, an uncertainty classification and quantification study was conducted. This study attempted to decompose two main sources of uncertainty, epistemic and aleatoric uncertainty, and compare the relative effects of each on the predictive uncertainty in alternative fuel data.

There are two main categories of uncertainty relevant to modeling inaccuracies. The first, epistemic uncertainty, also referred to as model uncertainty, arises when a model is given insufficient training data to learn the patterns present in the dataset and accurately map input to output. This issue is particularly relevant in composition–property modeling for SAFs, because only extremely limited datasets are available for newer fuels, in contrast to conventional fuels. Consequently, machine learning models can predict the properties for conventional fuels quite well, yet they perform poorly on SAFs. The other source of uncertainty is aleatoric uncertainty, also known as data uncertainty, which can arise from various events, such as low-resolution input data; inaccurate measurement techniques for the collection of model input data; and stochastic events, such as ignition delay, that introduce unresolvable noise into the model. Figure 7 outlines the process of building composition–property models, and the locations of epistemic and aleatoric uncertainty in the process.

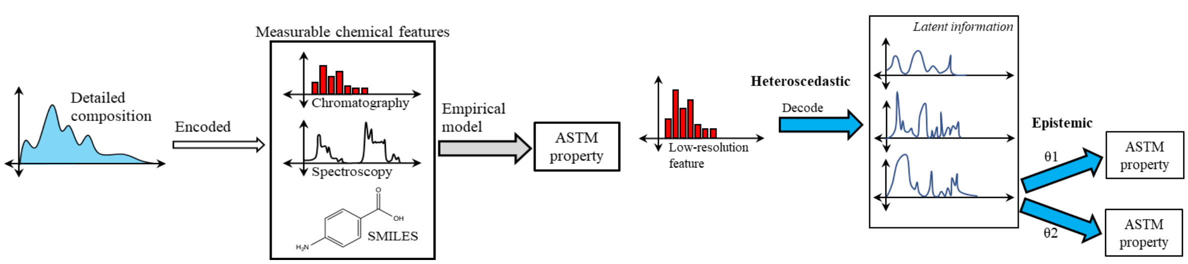

Figure 7. Schematic of SAF modeling, and epistemic and heteroscedastic uncertainties in this study.

To study the respective effects of each individual uncertainty type on the final model prediction for SAFs, we ran two separate computational tests, wherein epistemic and aleatoric uncertainty were induced artificially into the model, and the resulting uncertainty was calculated. To test epistemic uncertainty, we used three datasets with increasing SAF representation—and thus, theoretically, decreasing epistemic uncertainty—to build three separate probabilistic machine learning models. The performance of each model on the same test set of fuels was compared quantitatively. Figure 8 shows the test set of fuels used to assess the performance of each consecutive model; the black bars show data for the proxy fuels, thus demonstrating the qualitative chemical similarity of the proxy fuels introduced into each consecutive model compared with the test set fuel that the proxy fuel is meant to resemble. The test set was deliberately selected to be highly chemically diverse, to serve as a good indicator of model performance.

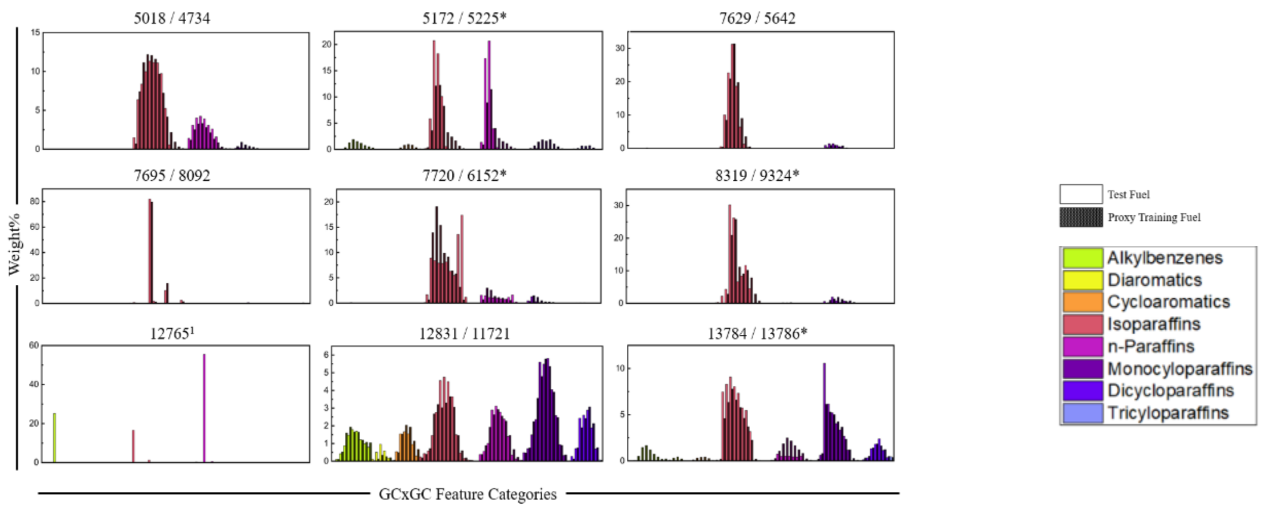

Figure 8. Summary of the test sample F68, juxtaposed with its proxy (black solid lines), with the exception of POSF 12765[1]. Pseudo-proxies are marked with an asterisk.

In this study, we were able to obtain quantitative results for the varying performance of each model on the same test set. Figure 9 represents the probability density functions for the predicted flash point values for each test set fuel according to each of the three machine learning models. The vertical lines represent the true value (experimental). In almost all cases, we were able to establish the anticipated result: the most diverse training set—D3, in blue—showed a shift in the peak of the probability density function closest to the actual value. In most cases, we observed that the distribution of the probability density function was narrower with increasing dataset diversity, thus translating to higher confidence in the predicted value at a higher accuracy.

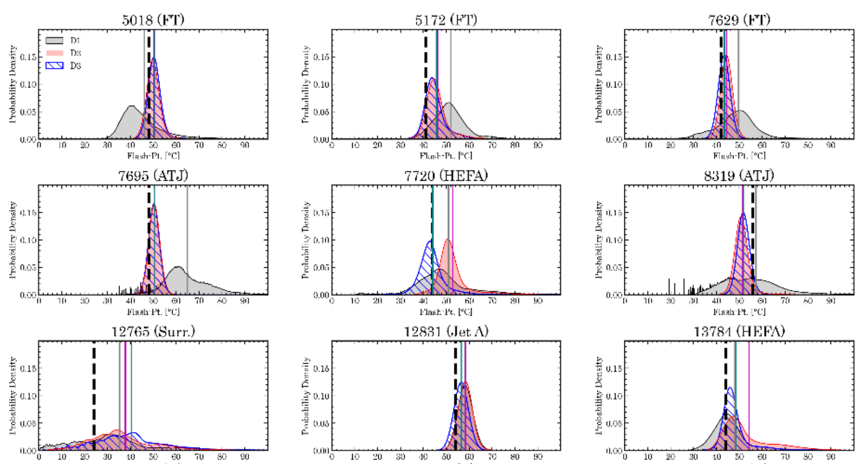

Figure 9. Predicted probability density functions using eBNN (explanation based neural network) with five hidden layers, trained on F68 and D1–D3.

The heteroscedastic (aleatoric) uncertainty was tested by artificially inducing lower-resolution data into a dataset with minimal epistemic uncertainty (one trained on only Jet A fuel, the most abundant fuel type), by summing the weight percentages in each subcategory of the 68 original GCxGC features in their respective chemical families. Through this process, and training two separate probabilistic models—one with 68 features and one with 8 compressed features—we observed a noticeable increase in uncertainty after feature compression (Figure 10). This uncertainty, indicated by the variance of the resulting predictions on the test samples, was then decomposed according to the law of total variance into its epistemic uncertainty and aleatoric uncertainty.

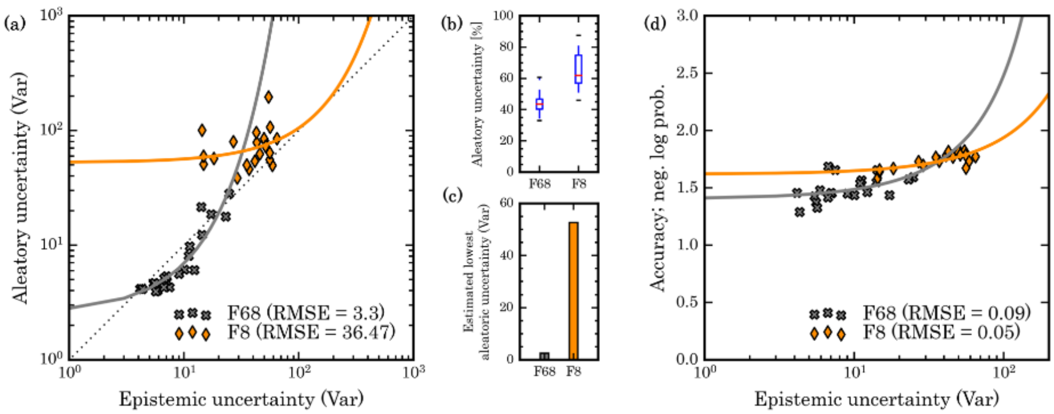

Figure 10. Uncertainty decomposition of POSF 12831, Jet A. (a) Epistemic versus heteroscedastic uncertainty. (b) Relative ratio (%) of heteroscedastic uncertainty of F68 and F8. (c) Minimum heteroscedasticity, estimated by the exponential fit of F68 and F8. (d) Accuracy (negative log probability of truth) versus epistemic uncertainty.

The results underscore the importance of generating and centralizing a more extensive dataset for SAFs for decreasing the uncertainty and thus increasing the confidence of predictive models for low-volume fuel prescreening. After sufficient data are generated and compiled, the bottleneck then becomes the resolution and subsequent reliability of the input and output data themselves. This bottleneck can be overcome through higher-fidelity laboratory testing and new experimental methods, such as vacuum ultraviolet radiation, which may potentially resolve the composition of single isomers within a given GCxGC bin.

Milestones

3 months

- Formalization of machine learning implementation plan

6 months

- Establishment of scripts and algorithms for implementation of machine learning
- Organization of target data from the database for implementation of machine learning

9 months

- Implementation and optimization of machine learning algorithms

12 months

- Finalization of all machine learning tasks for publication

Major Accomplishments

In the past year, work was undertaken to address the substantial issue of uncertainty in machine learning applications in this field of study. Outstanding obstacles were identified with respect to any future work in reducing uncertainties in the prescreening phases of new fuel certification. Machine learning applications such as these will be critical to advancing the prescreening and optimization process for new alternative jet fuels in the commercial sector. Neural networks were used to investigate confidence levels under various data circumstances to better understand their potential.

Publication

Peer-reviewed journal publications

Oh, J., Oldani, A., Lee, T., & Shafer, L. (2022, January 3). Deep neural networks for assessing sustainable jet fuels from two-dimensional gas chromatography. *Aerospace Research Central, AIAA 2022-0228*. doi: 10.2514/6.2022-0228

Outreach Efforts

The database has been made accessible through https://altjetfuels.illinois.edu/.

Awards

None.

Student Involvement

This project was conducted primarily by two graduate students (Ji Hun Oh and Alex Solecki).

Plans for Next Period

Moving forward, we anticipate that the machine learning component of this project will make up a less substantial portion of the efforts on this project. The focus will turn toward the development of the database and data collection, and the presentation of data from U.S. airports and international programs. Progress made to this point in the Machine Learning subtask will serve as a foundation for future case work on an "as-seen-fit" basis (see "Plans for Next Period" from Task 1).