Project 033 Alternative Fuels Test Database Library (Year III)

University of Dayton Research Institute, University of Illinois

*this report covers portion of University of Illinois

Project Lead Investigator

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- P.I.(s): Tonghun Lee, Associate Professor
- FAA Award Number: 13-C-AJFE-UI-009
- Period of Performance: 8/15/2016 to 8/14/2017
- Task(s):
    1. Development of an alternative fuels test database

Project Funding Level

Funding Level: $120K
Cost Share: Software license support from Reaction Design (ANSYS)

Investigation Team

- Kyungwook Min (Graduate Student, University of Illinois at Urbana-Champaign): Compilation of fuel test data.
- Anna Oldani (Graduate Student, University of Illinois at Urbana-Champaign): Compilation of fuel test data and development of database.

Project Overview

This study seeks to create a comprehensive, foundational database of current and emerging alternative jet fuels by integrating relevant pre-existing jet fuel data into a common archive which can provide guidelines for design and certification of new jet fuels in our future as well as aid federal work including fuel certification. Thus far, the effort has focused on the integration and analysis of pre-existing jet fuel data from various government agencies and individual research groups with oversight from the Federal Aviation Administration (FAA). We hope that the database will one day serve as 'the comprehensive and centralized knowledgebase' shared by the academic, government, and industrial communities in fuels research and policy, possibly facilitated on a cyber-based infrastructure. With ongoing prolific diversification of new jet fuels, this effort to integrate dispersed information is critical in providing the FAA with an overview of the latest developments and to support many other tangential fields of research in government, industry, and academia impacted by integration of new alternative jet fuels.

Task #1: Development of an Alternative Fuels Test Database

University of Illinois at Urbana-Champaign

Objective(s)

The main objective of this study is to establish a ***foundational database*** of current and newly emerging alternative jet fuels by integrating all relevant pre-existing jet fuel data into a common archive which can provide guidelines for design and certification of new jet fuels in our future as well as aid and shorten fuel certification relevant work. This proposal outlines the year II efforts under this mandate. The vision is to institute a database that can be utilized for the design and optimization of new propulsion and energy systems including development of next-generation engines, fuel delivery systems, as well as pollution mitigation technologies. Furthermore, it can provide data for screening and certification of newly emerging fuels and thereby impacting legislative measures and national policy. In so doing, the goals of this project are as follows:

- Survey current pre-existing data and analyze information
- Prioritize current data and compile into centralized logical structure
- Analyze the obtained information into chronological order and regroup into relevant groups
- Obtain information on detailed test platforms and test conditions
- Develop a controlled web portal for access to the information
- Develop and implement a database/web portal infrastructure and methodology
- Integrate available alternative fuel test data into the database in organized format
- (Future Work) Integrate FAA ASCENT and NJFCP Data

Research Approach

Development Strategy of a Successful Fuels Test Database (Long Term Plan)

- **Phase I:** Integrate Current Pre-Existing Data: Preliminary survey and integration of all pre-existing database and data (including raw data) on jet fuels from universities, national laboratories, government archives, and private industry (i.e., existing database from Sandia, NIST, DoD Labs, ASTM research reports, government technical reports etc. is part of the year I efforts and will be used to initially seed the basic infrastructure of the fuels database proposed in this study). Year II efforts continued to assemble information and annex a prioritized set into the web portal/database. In year II, we focused our efforts on obtaining relevant fuel property specification test data for the certification process.
- **Phase II:** Analysis of Preliminary Data: Conduct comprehensive analysis of the initial data to categorize all relevant physical and chemical characteristics of the fuels and relevant testing conditions. Effort will be made to determine insufficient areas for further investigation. In year II, we have significantly expanded our efforts to the analysis of information into chronological order and in incorporating detailed test platform and test condition data. An effort will be made to re-categorize the data according to different testing groups and performance. A preliminary effort will be made to vet some of the data according to test conditions as required (future efforts will more fully address vetting and analysis of data).
- **Phase III:** Establish Web Portal/Database Infrastructure and Methodology: A basic web portal has been established during the year I efforts. In year II, based on the analysis of pre-existing data, we will work with national laboratories to establish a flexible and accessible database structure and data access protocols both for retrieval of current data and also for integration of new information in the future. This will be integrated into the web portal. We anticipate increased functionality in the web portal to conduct advanced searches and user feedback on each data item (community based vetting system).
- **Phase III-b:** Integration of FAA ASCENT and NJFCP Data: New data generated from both the FAA ASCENT and the NJFCP will be integrated into the database according to the pre-defined infrastructure. This will be coordinated with Area #7 of the NJFCP program.
- **Phase IV:** Integrate with Current and Future Research: Disseminate and integrate new database to relevant research groups in universities, national laboratories, government, and industry. Formulate partnerships for stewardship, preservation, and continued development of the alternative jet fuel database to include emerging analysis methods (e.g. GCxGC fuel analysis).
- **Phase V:** Continued Development: Continue development of the database after the initial integration and distribution phase into a more widely distributed community based infrastructure (potentially cyber-based). Link and expand the database to encompass pre-existing data from other countries as well as interlink with efforts such as Europe's JETSCREEN program.

Milestone(s)

Milestone 1 (up to 10/1/2016)

Proposed: The first milestone of this reporting period was to complete the technical development of the database site housed at the University of Illinois with user registration and other additional requested features including refinement of the search results and data categorization. We will also continue to visit AFRL to obtain fuel test data for inclusion on the site as well as other relevant fuel reports and publications.

Achieved: We finalized the design and organization of the website housing the Alternative Jet Fuels Test Database Library. We are confident that this final structure achieves the needs and features identified by the jet fuel community. Additional data retrievals were completed during this period to obtain testing data for approved alternative jet fuels that have been annexed under ASTM D7566 including FT, HEFA, SKA, SIP, and ATJ.

Milestone 2 (up to 12/1/2016)

Proposed: For our second planned milestone, we will determine the feasibility of including the chemometric analysis software developed by NRL, FCAST, into the database. This will involve an evaluation of the software and its potential usefulness for alternative jet fuel development partners. We also plan to reach out to link in additional related programs dealing with aviation industry such as CLEEN, CAAFI, and NJFCP.

Achieved: We obtained a license from NRL to use the FCAST software at the University of Illinois to evaluate its potential use within the database. With this access, we ran sample alternative jet fuel data to determine how well the FCAST software performed in its fuel property predictions. It performs a Partial Least Squares (PLS) regression to establish correlations between measured fuel chemical components and observed fuel properties from a test dataset. It then uses these correlations to provide fuel property predictions of relevant aviation fuel specifications. We also tested the blending feature of the software, which allows users to blend the GCxMS data of two fuels in 10% increments. After analyzing the software, we determined it could be implemented at some future point into the database if there is enough support to fund such a project. However, in its current state, FCAST is a standalone software that would require modification to be integrated into an online portal such as the database. Regarding additional related programs, we continued conversations with groups involved in the NJFCP program to assess if the AJFTD site could serve their needs. We agreed to function as data and documentation dissemination site as specified under the Data Management Plan for the NJFCP program. Further discussions will be ongoing to determine the appropriate timing and release of data.

Milestone 3 (up to 12/31/2016)

Proposed: To wrap up 2016, we will conduct an initial survey of alternative fuel properties taken from the AFRL fuels database maintained at Wright-Patterson Air Force Base in Dayton, OH. This survey will help identify data still needed across the various alternative jet fuel categories. We will also discuss with our AFRL collaborators useful next steps to take regarding data collection and analysis.

Achieved: After examining the initial retrievals of fuel test data (primarily from AFRL), we decided to task ourselves with collecting additional fuel data for the HEFA and ATJ fuel categories. We also began discussions regarding future directions of fuel analysis, specifically potential improvements to current testing methods. This also began our discussions with project collaborators dealing with the ASTM Generic Annex proposal to evaluate how the AJFTD site can support the goals to streamline the certification process for new alternative fuels.

Milestone 4 (up to 3/31/2017)

Proposed: For the first quarter of 2017, we will begin to develop a statistical analysis of fuel variation data taken from reports such as the World Fuel Survey and alternative fuel approval reports. From these data sources, we will evaluate property-temperature relations for properties including density, viscosity, isentropic bulk modulus, and surface tension. We hope to determine whether significant variance exists in property temperature dependence between conventional and alternative jet fuels.

Achieved: Following our discussions with project collaborators at the NJFCP meeting, we obtained fit for purpose fuel property data that allowed us to analyze the variance of the aforementioned properties with regard to temperature. From this analysis, we concluded that across all properties, several alternative fuel categories show significant variance from conventional fuels.

Milestone 5 (up to 5/31/2017)

Proposed: For the next milestone, we will work to evaluate the implication of the variance observed in the alternative jet fuels. We will seek to determine if the significant variability of alternative fuels from conventional fuels poses additional considerations for the ASTM Generic Annex. To accomplish this, we will develop expected fuel property ranges from the fuel variance data and then compare these expected ranges with specification requirements.

Achieved: Using the fuel variability data, we generated 95% confidence intervals to provide expected fuel property ranges to evaluate if, given their variability, the alternative fuels remain within specification requirements. We concluded that, for all properties evaluated, the alternative fuels remain with specification requirements as outlined in ASTM D7566. This provided us with the assurance that alternative fuel variability does not present an additional concern for meeting fuel specifications.

Milestone 6 (up to 8/14/2017)
Proposed: For the final milestone of this reporting period, we will evaluate whether FCAST can be used to support the proposed requirements under the ASTM Generic Annex. Specifically, the Generic Annex seeks to introduce new alternative fuels at low blending ratios of 10%. To provide justification for this blending level, we will test the blending capability of FCAST by comparing the fuel blend tool with actual blended fuel results. Following this, we can determine the accuracy of FCAST in computing fuel blend properties using solely fuel blend-stock data without utilizing actual blended fuel data.
Achieved: We worked with FCAST to test blends of A1 (JP8) and C1 (Gevo) fuels in in varying ratios. We evaluated the FCAST blending tool by providing GCxMS data for the neat components and blending within the tool to then predict property values. We compared these blend predictions with actual blends of A1 and C1 that were prepared and run through our GCxMS facility. The data from these actual blends was then provided to FCAST to compute predicted properties. In comparing the predicted properties for the computed blend and the actual blend, we found less than a 5% difference across most properties for all the fuel blends. From this, we concluded that the FCAST blending tool does an accurate job at predicting blended fuel properties, and thus, can be potentially used to evaluate fuel blends for the ASTM Generic Annex.

Major Accomplishments

The Alternative Jet Fuels Test Database, established through the coordinated efforts of members at the University of Illinois, continued to grow with additional jet fuel test data, which was utilized for a statistical analysis of fuel variability during year III. Improvements over the years include the development of basic and advanced search functionalities and enhanced search algorithms to return more robust search results. There are public access areas including general information regarding the mission and goals of the database project, funding agencies of the program, a directory of members involved in the work, and links to partner institutions participating in the larger FAA ASCENT database project, links to relevant updates regarding alternative jet fuel, and links to contact site administrators. There are also site features accessible only to registered users that include links to the advanced and basic search features of the database, access to the database file dropdown feature, and descriptive information of the various areas under the NJFCP program which will include NJFCP data in the future. To register, users must request access and be approved by site administrators. Registered users can also submit data directly to the site, which is reviewed and categorized by site.

Users have two methods to access data on the site: a basic or advanced search which allow users to search by terms of interest (e.g. authors, title, DOI, year of publication, data type, and keywords) and file folder dropdown structure that gives users access to all the categorized documents without requiring users to input a specific search term. Users can download original file formats as well as any tabular data that has been converted into .XLSX files for improved accessibility. The site will also house data from the National Jet Fuel Combustion Program (NJFCP) Areas 1 through 6. Discussions are ongoing as how to best to include data from this multi-group collaborative effort. Once further guidelines have been discussed and approved regarding which data to include, this section of the site will be expanded.

In year III, the data contained within the database was analyzed for variability of thermophysical properties. This work was done to provide a more thorough understanding of the variation present in alternative jet fuels. A statistical analysis of conventional fuels and alternative fuels approved via annexation to the ASTM D7566 Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons found significant variance in property-temperature relations for alternative fuels as compared to World Fuel Survey conventional fuel averages and is summarized in Table 1. The full results for slope and intercept results with slope statistical analysis results are shown in Table *2* for the alternative fuel categories as compared to conventional fuels. Bolded results indicate properties that are significantly different from conventional fuels (WFS) while statistical tests were not done on pure hydrocarbons (HCs, HCs1, HCs2) or CRC handbook properties (CRC).

Table 1: Summary of property-temperature relation variance

Fuel Property	*Fuels with Significant Variance*
Density	SKA
Isentropic Bulk Modulus	HEFA, FT
Specific Heat	FT, FSJF
Speed of Sound	HEFA
Viscosity	SKA, HEFA

Table 2: Property-temperature relation variance results

Density	*Slope*	*Intercept*	*T-test*
WFS	-0.7216	815.49	
WFS w. light+heavy	-0.7225	815.53	
FT	-0.7376	777.68	0.0778
SKA	-0.7439	796.76	**0.0239**
Renewable	-0.7419	796.87	0.1694
HCs 1	-0.8881	826.87	
HCs 2	-0.8651	825.48	
CRC	-0.7723	817.66	

Specific Heat	*Slope*	*Intercept*	*T-test*
WFS	0.0036	1.5597	
FT	0.0030	1.7845	**0.0466**
FT 2	0.0032	1.7732	0.0763
FSJF	0.0018	1.5797	**4.7E-06**
HEFA	0.0037	2.0513	0.4214
2nd Gen	0.0037	1.8663	0.8462
HCs	0.0042	1.7836	
CRC	0.0035	1.7233	

Speed of Sound	*Slope*	*Intercept*	*T-test*
WFS	-4.113	1403.7	
FT	-3.974	1399.4	0.0686
HEFA	-2.748	1371.4	**0.0010**
HCs	-3.641	1339.6	

Viscosity	*m*	*b*	*T-test*
WFS	0.9750	2.8487	
FT	0.9758	2.9994	0.7989
SKA	0.9815	3.0912	**0.0015**
HEFA	0.9777	2.8944	**0.0137**
2nd Gen	0.9708	3.2623	0.3013
HCs	0.9890	1.8502	

Where: $y=bm^x$

Surface Tension	*Slope*	*Intercept*	*T-test*
WFS	-0.0751	27.407	
FT & HEFA	-0.0741	25.921	0.8581
SPK	-0.0800	25.873	0.2261
Renewables	-0.0771	26.687	0.4125
CRC	-0.0443	15.971	

To evaluate the impact of this variance, 95% confidence intervals were constructed from the fuel data to provide expected property value ranges for the various properties evaluated including density, isentropic bulk modulus, specific heat, speed of sound, and viscosity. It was important to assess whether the significant variance as identified from **Table *2*** would result in property values that do not meet specification requirements. From these property value bounds, it was concluded that the fuels remain within specification requirements for the properties under consideration. Averaged property-temperature relations were also produced for the examined fuel categories and are shown in **Table *3***. These averaged relations can be used to provide property ranges for the various fuels categories, useful for determining property values that can be reasonably expected for each respective fuel category. When evaluating fuel blends for the ASTM Generic Annex, similar property-temperature relations can be constructed to provide the bounds for possible fuel properties. These relations can then be analyzed as blend ratios vary, to determine the magnitude of the impact of blend ratios on resulting fuel properties, specifically properties identified under fuel specification requirements.

Table 3: Averaged property-temperature relations

Density	*Equation*
WFS	y=-0.7216x +815.5
WFS w. light+heavy	y=-0.7225x +815.5
FT	y=-0.7376x +777.7
SKA	y=-0.7439x +796.8
Renewable	y=-0.7419x +796.9
HCs 1	y=-0.8881x +826.9
HCs 2	y=-0.8651x +825.5
CRC	y=-0.7723x +817.7

Specific Heat	*Equation*
WFS	y=0.0036x +1.560
FT	y=0.0030x +1.784
FT 2	y=0.0032x +1.773
FSJF	y=0.0018x +1.580
HEFA	y=0.0037x +2.051
2nd Gen	y=0.0037x +1.866
HCs	y=0.0042x +1.784
CRC	y=0.0035x +1.723

Isentropic Bulk Modulus	*Equation*
WFS	y=-10.715x +1629
Boeing HEFA	y=-7.957x +1720
FT	y=-9.864x +1603

Speed of Sound	*Equation*
WFS	y=-4.113x +1403.7
FT	y=-3.974x +1399.4
HEFA	y=-2.748x +1371.4
HCs	y=-3.641x +1339.6

Surface Tension	*Equation*
WFS	y=-0.0751x +27.4
FT & HEFA	y=-0.0741x +25.9
SPK	y=-0.0800x +25.9
Renewables	y=-0.0771x +26.7
CRC	y=-0.0443x +16.0

Thermal Conductivity	*Equation*
Renewables	y=-1.43E-04x +1.16E-01
FT	y=-4.72E-05x +1.34E-01
FSJF	y=-3.11E-07x +2.98E-04
HEFA	y=-8.52E-05x +1.05E-01

Viscosity	*Equation*
FT	y=2.999*0.9758x
SKA	y=3.091*0.9815x
HEFA	y=2.894*0.9777x
WFS	y=2.849*0.9750x
2nd Gen	y=3.262*0.9708x
HCs	y=1.850*0.9890x

Finally, work was also completed in collaboration with NRL and their fuel chemometric analysis program, FCAST. This software performs a Partial Least Squares regression analysis to correlate fuel composition to expected specification properties. Using a training set of data, these correlations can then be applied to new GCxMS data provided to the program, resulting in predicted properties for jet fuel relevant specifications. We were granted access to this software, allowing us to evaluate its performance for alternative aviation fuels. We also employed the fuel blending tool to assess the potential for its use to support the ASTM Generic Annex approach of introducing new alternative fuels at lower blending ratios of around 10%. To evaluate the blending capability, fuel samples of A1 (JP8) and C1 (Gevo) fuels were prepared as neat samples and blended mixtures of varying ratios. **Figure *1*** shows the results of a 50:50 A1:C1 fuel blend as calculated by the FCAST blending tool and as prepared in the lab. When the predicted fuel properties of the calculated blend and actual blend are compared, generally a 5% or less difference is observed for all properties at the varying blend ratios. We believe that this tool can support the plans within the Generic Annex to provide control of conventional and alternative fuel blends through limited alternative fuel blending levels. Additionally, if there is interest in the future to integrate an FCAST type tool on the AJFTD site, modifications can be made to its current form to allow for online accessibility.

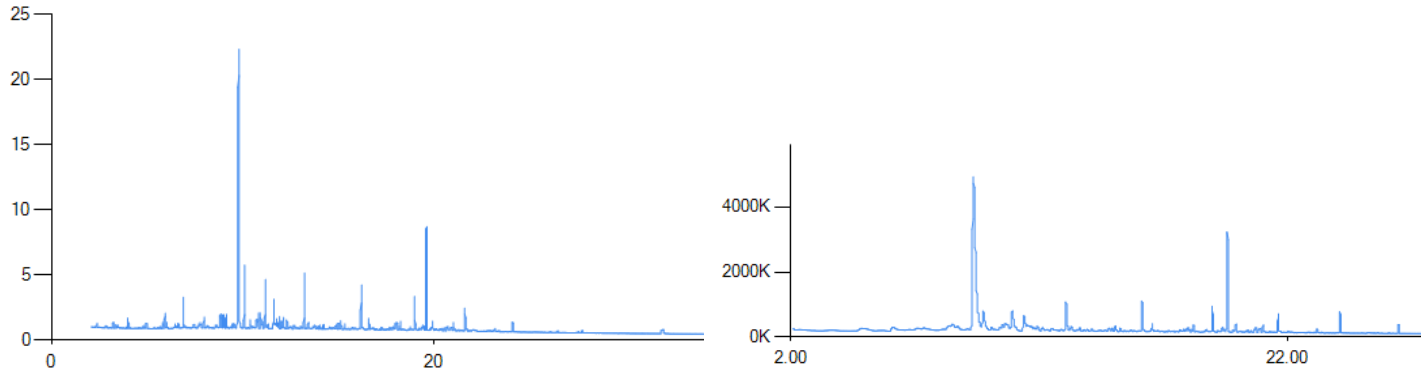

Figure 1: 50:50 A1:C1 blend - calculated TIC (L), actual TIC (R)

Publications

(In Progress) Oldani, Anna. "Alternative Jet Fuel Variation and Certification Considerations." 2017.

Outreach Efforts

None

Awards

Anna Oldani (Graduate Student): Society of Women in Engineering (SWE) Award for Research Excellence

Student Involvement

Two graduate students (listed above) have participated in this project on a rotational basis to address various aspects of the project. They have surveyed the data, interacted with the data sources and created strategies to integrate the data into the database. They developed the web-based portal for the actual implementation of the web interface. They have also conducted a statistical analysis of the available data to evaluate property variance. They continue efforts to update the database with relevant alternative jet fuel test data as it is made available.

Plans for Next Period: Start of Analysis

Year IV for the database project will see continued evaluation of the data contained within the database as well as an assessment of emerging fuel analysis methods such as GCxGC. Several key efforts are planned and are currently underway. They include:

- Evaluation of GCxGC procedures and data processing methods
- Inclusion of available GCxGC data for approved alternative jet fuels to the database site
- Data analysis of fuel blending ratios to support ASTM General Annex effort for fuel certification to determine additional correlation work to link fuel properties to the overall evaluation
- Inclusion of NJFCP data: put up vetted and organized NJFCP data on the database
- Integration of efforts with European JETSCREEN program to collaborate fuel screening and property evaluation under NJFCP program