Project 33

Alternative Jet Fuel Test Database Library

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PM: Prem Lobo

Cost Share Partner: Ansys, Inc.

Objective:

This project's objective is to establish a comprehensive and foundational database of current and emerging alternative jet fuels by integrating relevant new and pre-existing jet fuel test 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. Currently, we are in the process of connecting our database with European projects ALIGHT and NewJET as well as setting up live, periodic fuel data sampling from domestic airports across the US. Additionally, we are looking to leverage existing data and machine learning techniques to support development of prescreening and kinetic analysis tools for new fuels undergoing the rigorous and resource intensive certification process.

Project Benefits:

Further development of a centralized alternative jet fuel test database with a broad range of data categories and extensive sampling under each data type would benefit fuel scientists and researchers investigating variability of new fuels, composition-property relationships, engine operability metrics, cost of production, production methods, fuel storage and transportation methodology and design, etc. This in turn will benefit policy makers and shareholders in making informed decisions in the integration of AJF into the commercial sector. At the high level, this database ultimately provides a critical foundation for the implementation of AJF and will assist in achieving new climate and sustainability targets in the sector as they become more demanding in future policy.

Research Approach:

Develop a Comprehensive SAF Database on Properties & Testing

- Assemble data into a centralized database for sustainable aviation fuels
- Apply advanced analysis technique: Machine-Learning based strategies
- Enhance website usability and analysis functionalities
- Connect database to international network: ALIGHT and NewJET
- Forge a new data pipeline with domestic US airports: fuel test data reports
- Incorporate a variety of testing data beyond composition-property test reports

In anticipation of 100% SAF efforts being realized and unprecedented politico-financial support supplied for the testing and scaling of new sustainable aviation fuels and blend stocks, two main actions become paramount: (1) Accurate and regionally specific tracking and monitoring of jet fuel composition, property, blending and usage trends, and (2) improved methodologies for rapidly assessing both chemical-property and engine operability indicators for newer fuels undergoing the certification process. With a rapidly diversifying landscape of alternative fuels and increased momentum in national integration efforts, the need for close monitoring and analysis of the state-of-the-art in AJF becomes critical in proceeding with ultimate SAF adoption under high levels of certainty and control.

Major Accomplishments (to date):

Accomplishments in Current Year

- Improved online interface, data retrieval and analysis functionalities
- Assessed obstacles and solidified plans for domestic airport data pipeline
- Established contact with new international programs for data sharing
- Developed machine learning based techniques for fuel data analysis: Data imputation, uncertainty quantification and characterization, optimization frameworks for rapid kinetic mechanism model development

Future Work / Schedule:

- Continue data collection from pre-established fuel data sources
- Improve the online database usability and supporting features for analysis
- Detail data types and retrieval mechanisms from US airports
- Commence data sharing with ALIGHT and NewJET programs
- Expand test data scope to include contrail and emissions testing data
- Potentially incorporate LCA reporting on sustainability of new fuels per CORSIA, CLEEN, other third party organizations
- Further investigate the potential for building rapid kinetic models using composition-property data and novel machine learning frameworks

This research was funded by the U.S. Federal Aviation Administration Office of Environment and Energy through ASCENT, the FAA Center of Excellence for Alternative Jet Fuels and the Environment, project 33 through FAA Award Number 13-C-AFJE-UI-026 under the supervision of Prem Lobo. Any opinions, findings, conclusions or recommendations expressed in this this material are those of the authors and do not necessarily reflect the views of the FAA.

Background, Motivation, History

Principal Investigator: Tonghun Lee

Graduate Students: Alex Solecki, Ji Hun Oh

Research Approach

- **Assemble jet fuel test data** into an accessible, public database
- **Track jet fuel property trends** across the aviation fuel landscape
- **Establish a foundation** for SAF and alternative jet fuel research, certification and policy-making
- **Leverage global jet fuel data** to develop a real-time understanding of jet fuel variability as new fuel integration accelerates

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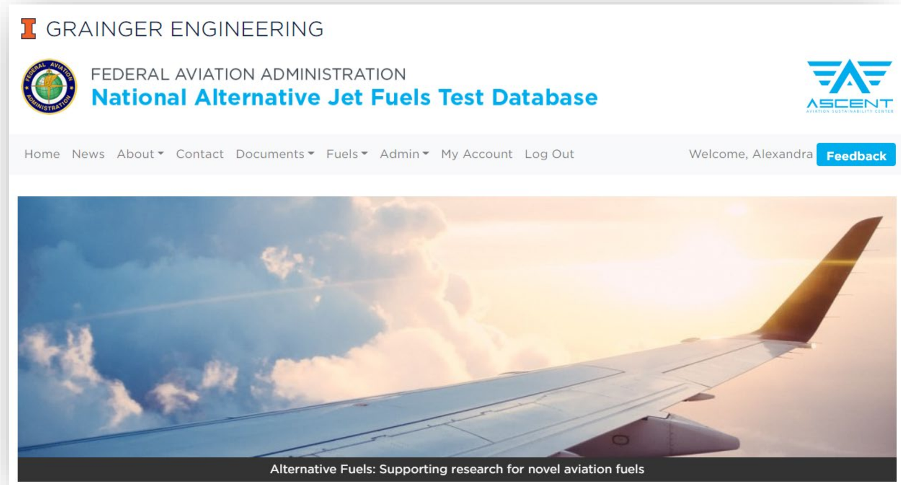

Figure 1. AJFTD website home screen.

NIST Ansys Honeywell

Rolls-Royce Williams International

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Background, Motivation, History

Data Sourcing: JETSCREEN, ALIGHT, NewJET

- **JETSCREEN** Screening and Optimization (2017 – 2020)
- **ALIGHT** Lighthouse Airports (2020 – 2024)
- **NewJET** New fuel specification (2040)

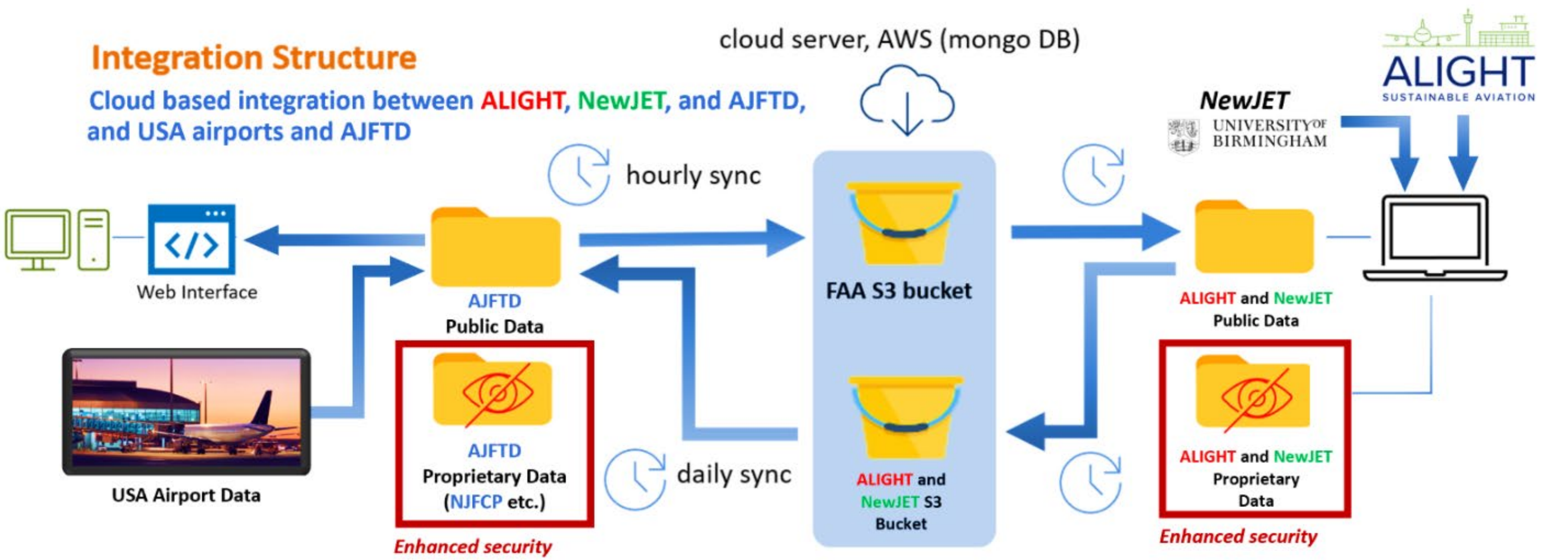

Figure 2. Data transfer infrastructure for domestic and international fuel data incorporation.

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Ongoing Data Acquisition

Domestic Airport Data Pipeline

Key Objectives

Real-Time Data Sampling

Emissions Monitoring

New World Fuel Survey

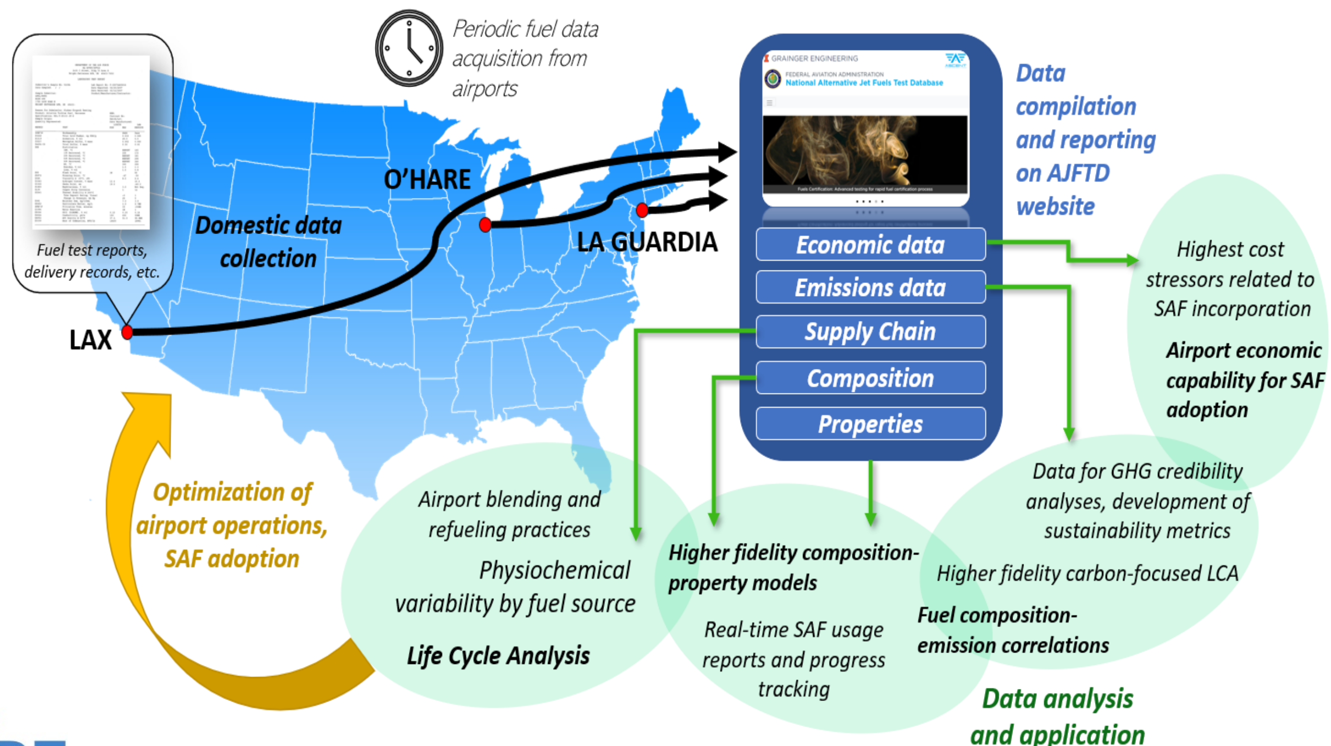

Figure 3. Domestic airport fuel test data integration and proposed applications.

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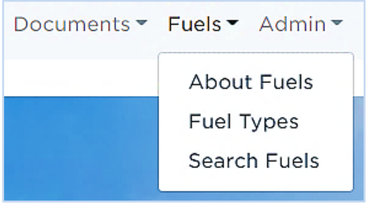
Website Updates

Alternative Jet Fuels Test Database Website Updates

- **Enrich** site usability and interface
  - New “About” pages
  - Feedback portal
  - Bug fixes and graphic cleanups
- **Organize** and clarify data tags for retrieval
  - Data retagging: Mass Python-JSON editing
  - Fuel type, classes, origins, descriptions
- **Expand** analysis tools and functions
  - New search categories
  - Mass compare function in progress
- **Connect** to network for AJF advancements
  - Link to CLEEN, CORSIA, participating airports
  - Documents → Publications, News



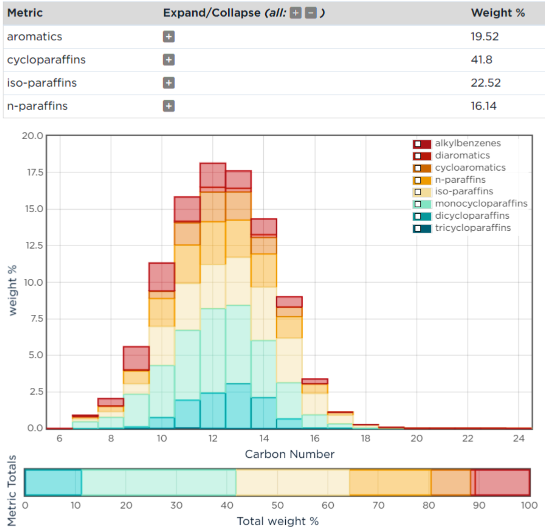


Figure 4. GCxGC Data interactive viewing.

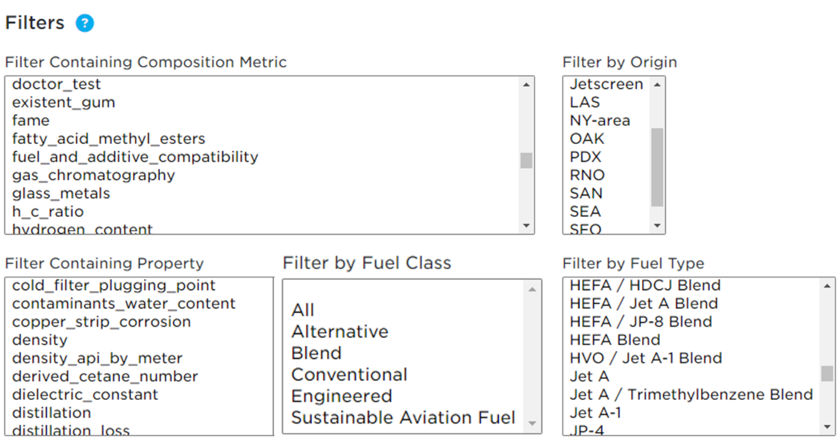


Figure 5. Fuels search page; search filters.

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Data Applications: Rapid Prescreening

Machine Learning and Prescreening

Property-Composition Data and Predictive Modeling

- **ASTM certification** is rigorous and resource intensive
- **Prescreening** methods can help reduce risks
- **Novelty detection** can assist in new fuel prescreening
- **Machine Learning Deep Neural Networks (DNN's)** used to detect outlying fuels at low volumes

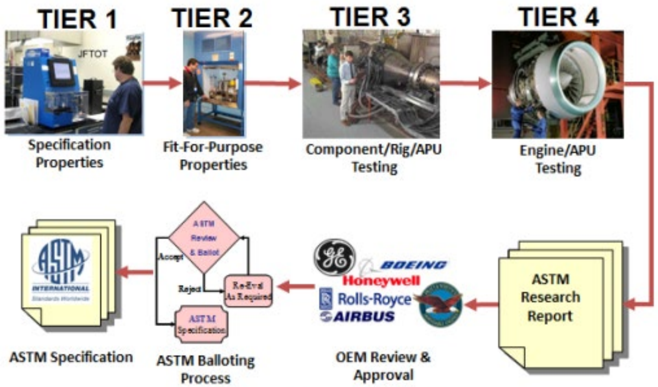

Figure 6. ASTM D4054 Certification Process.

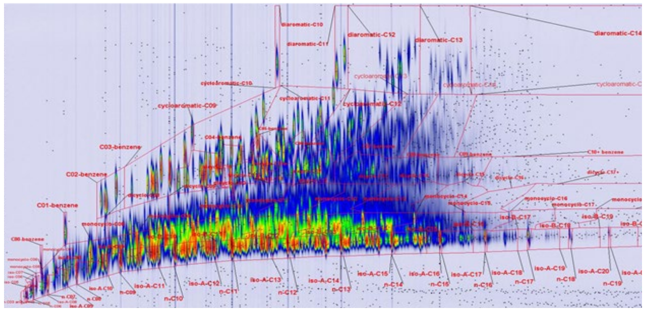

Figure 7. Sample of GCxGC chromatogram of corn syrup derived RPN/HDO-SK.

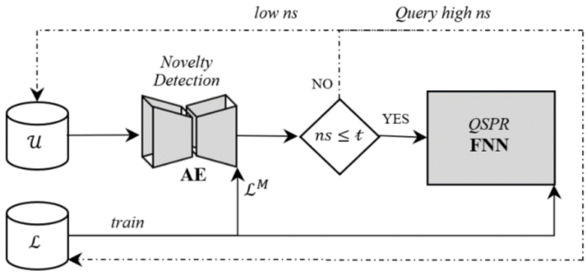

Figure 8. Schematic outline of proposed fuel novelty detection framework.

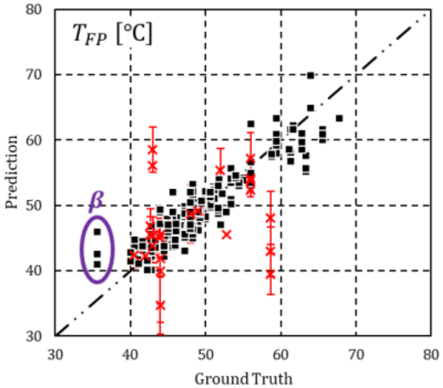

Figure 9. Regularized deep neural network fuel classifier.

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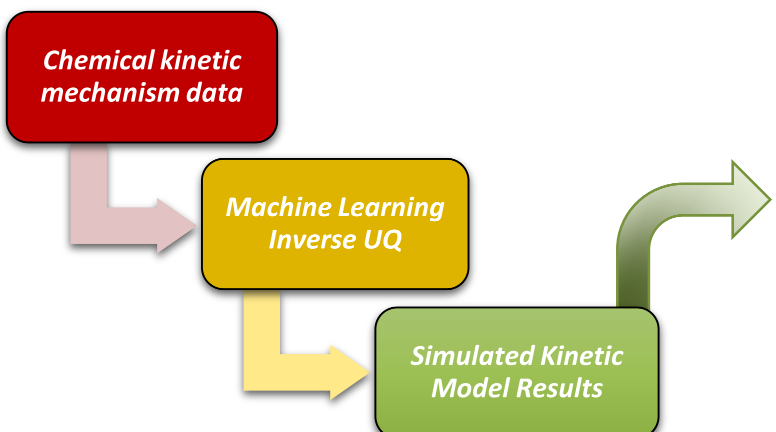
Data Applications: Rapid Prescreening

Machine Learning and Prescreening

Novel, Rapid Kinetic Mechanism Modeling

- **New fuel kinetic models** are time consuming to construct and validate
- **Inverse UQ** can be leveraged to learn kinetic model data and predict coefficients
- **IDT computational time reduced** significantly with assistance of ML model



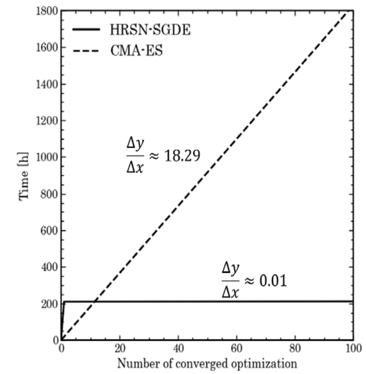


Figure 10. Computational time versus the number of obtained optimization results attained using HRSN-SGDE and CMA-ES.

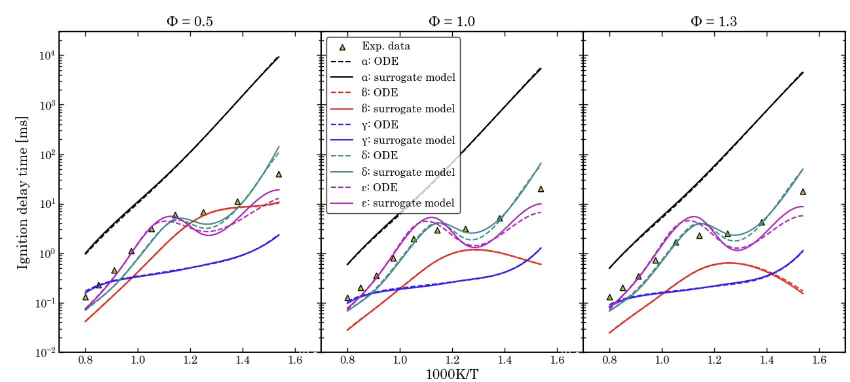


Figure 11. IDT's simulated (dashed) and predicted from the global surrogate (solid) for Jet A-CN40. Five test samples, α, β, γ, δ, and ε are plotted.

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Uncertainty Quantification (UQ)

Significance of Uncertainty in Prescreening and Fuel Testing

- Arises from novel fuel compositions and test data inaccuracies
- Translated risk of investment for producer / candidate

Uncertainty classification and quantification

- Increase confidence in prescreening results
- Identify types and sources of uncertainty for reduction

Uncertainty Quantification Study

- Classify and quantify sources of uncertainty in SAF composition-property modeling

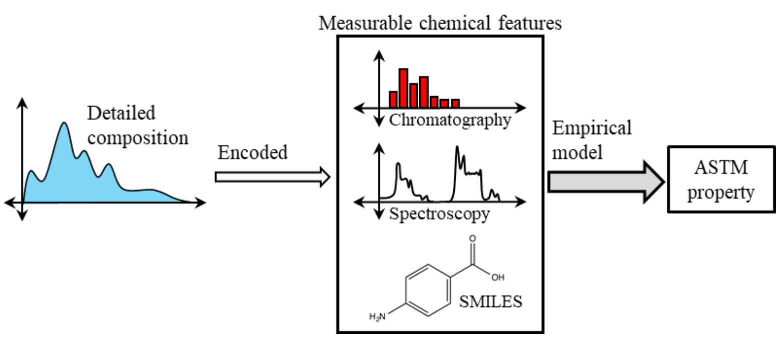

Fig 12. Schematic of empirical SAF property modeling.

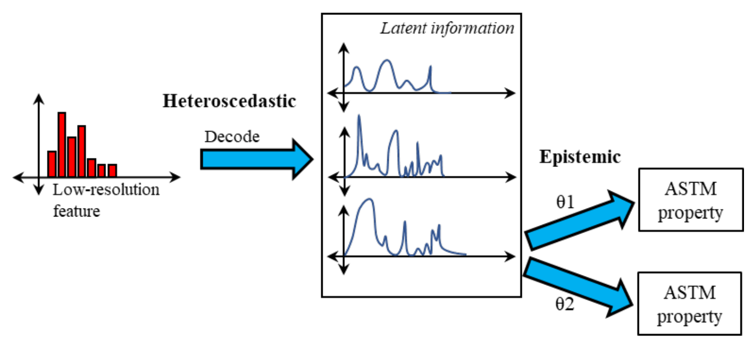

Fig 13. Epistemic and heteroscedastic uncertainties considered in this study.

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Uncertainty Quantification (UQ)

Dataset Generation AJFTD

- Three datasets generated of varying diversity
- Pseudo-proxy fuels included to test ability to reduce uncertainty with similar chemical representation
- Ensemble Bayesian Neural Network built to investigate behavior in overconfident – but uncertain - models

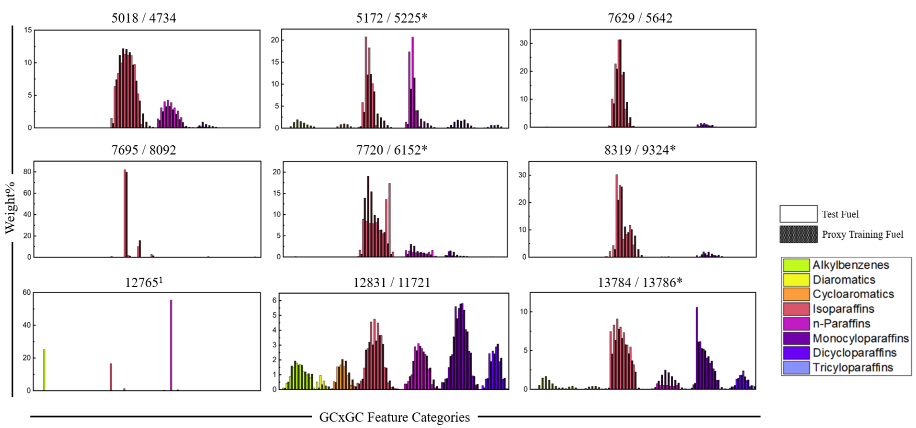

Figure 14. Summary of the test samples F68, juxtaposed by its proxy (black solid lines) with the exception of POSF 12765[1]. Pseudo-proxies are marked with an asterisk.

Aleatoric and Epistemic Uncertainty Results

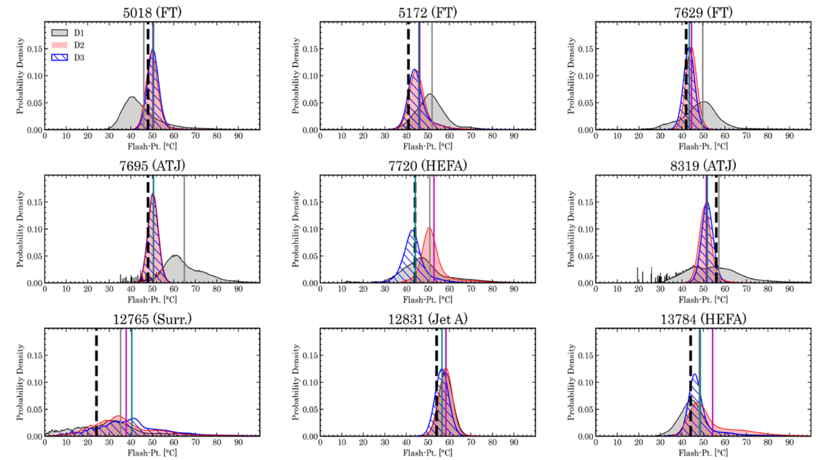

Figure 15. Predicted PDFs using eBNN with five hidden layers, trained using F68 and D1 to D3. Ground truth properties are plotted in dashed black lines. Mean of each PDF: solid gray, magenta, and teal lines for D1-D3.

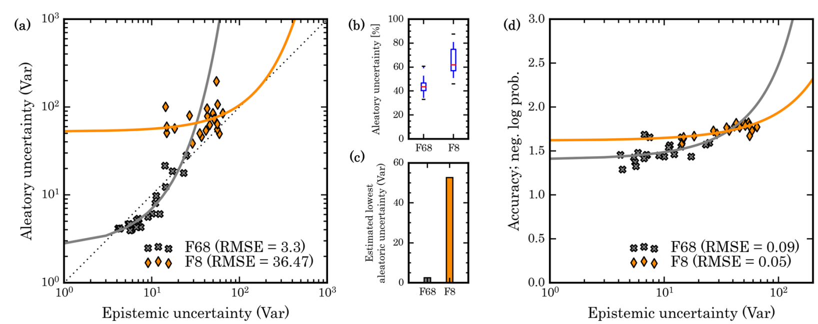

Figure 16. Uncertainty decomposition of POSF 12831, Jet A.

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Future Work

Emissions and Contrail Studies

- Altitude test chamber
  - Diagnostics for crystal formation and characterization
  - Incorporation with soot studies on M1 combustor
- Integration of emissions data into AJFTD
  - Support future wide-scale emissions tracking efforts

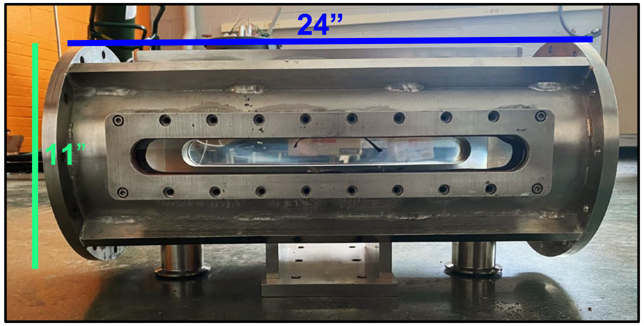

Figure 17. Candidate Test Chamber, Side View.

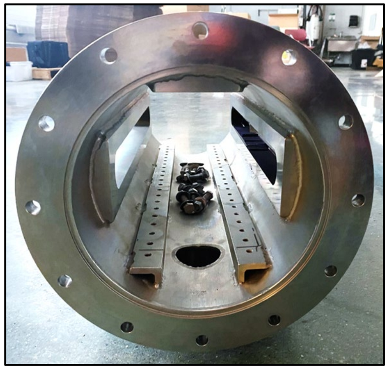

Figure 18. Candidate Test Chamber, Axial View.

Life Cycle Assessment Incorporation

- Aviation fuel sustainability metrics, research, data
- Centralize most recent LCA data across third party organizations

Domestic and International Data Sharing

- Initiate domestic airport, ALIGHT, NewJET data sharing
- Implement data pipeline infrastructure and transfer

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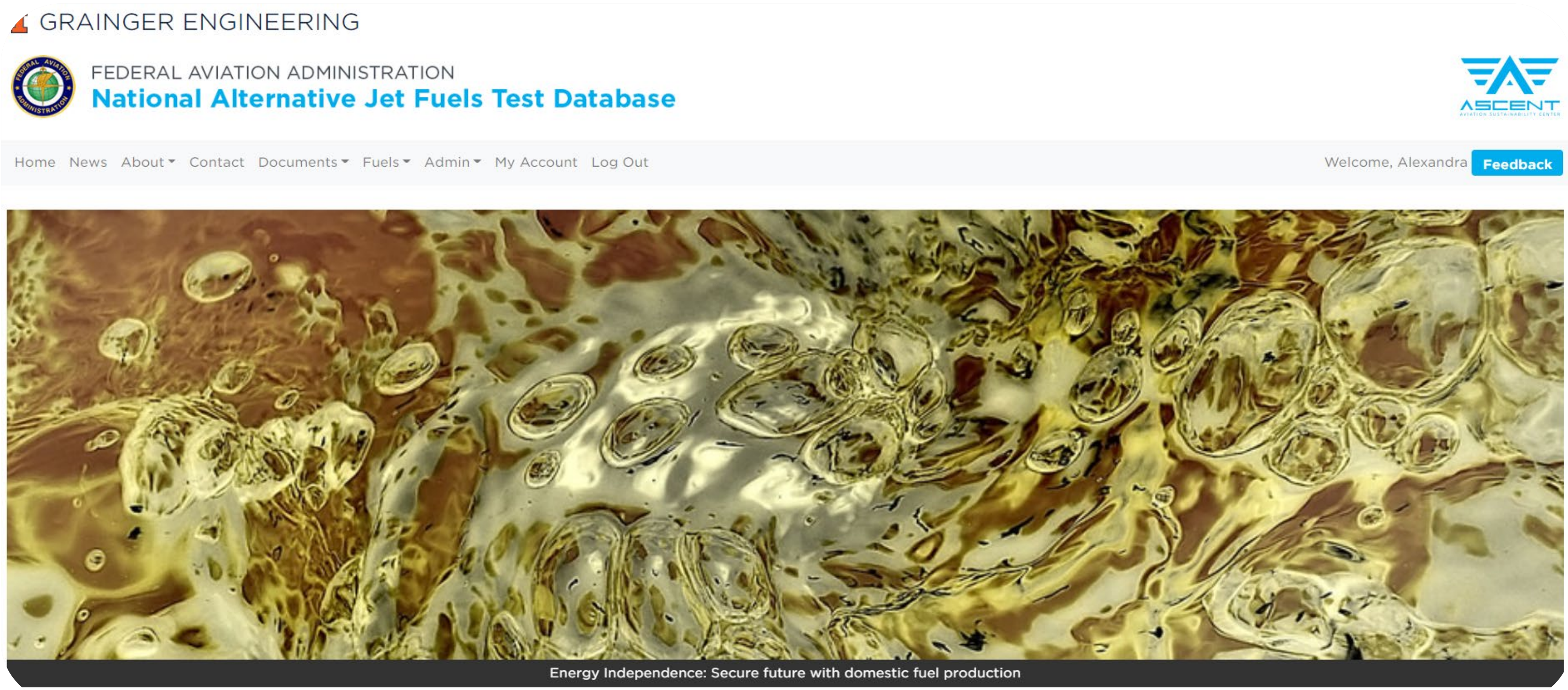
P33 Alternative Jet Fuels Test Database



Thank you!

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