

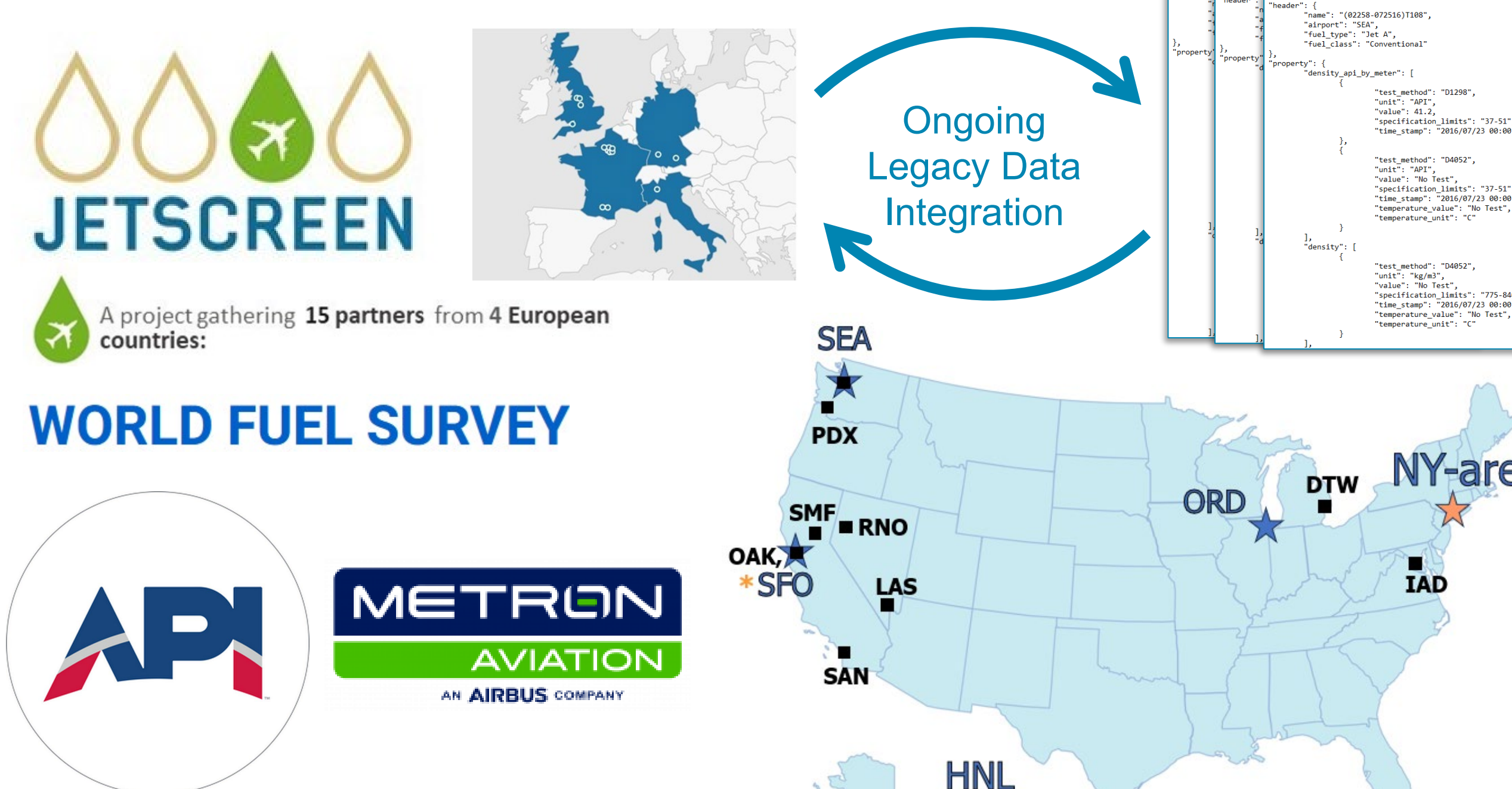
## Motivation and Objectives

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 synthetic fuels becomes critical. Proceeding with synthetic and alternative fuel adoption under high levels of certainty and control requires two objectives:

1. Accurate and regional specific tracking and monitoring of jet fuel composition, property, blending and usage trends
2. Improved methodologies for rapidly assessing both chemical-property and engine operability indicators for new fuels undergoing the qualification process

## Summary

**Maintain and expand jet fuel data archive** to establish a foundation for synthetic and alternative jet fuel research



## Results and Discussion

### A Comprehensive SAF Database

- Assemble data into a centralized database for synthetic aviation fuels and 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

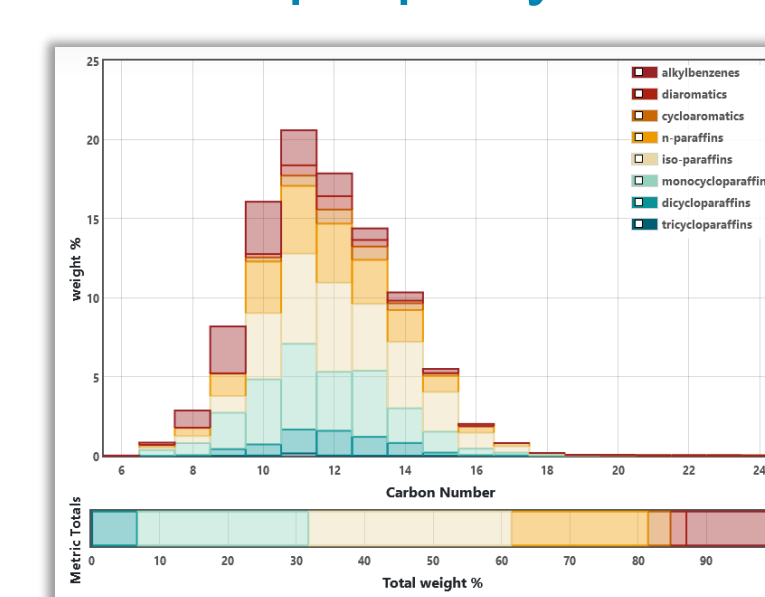
**NewJET:** a virtual center of excellence linking the chemical properties of a fuel to improved performance properties



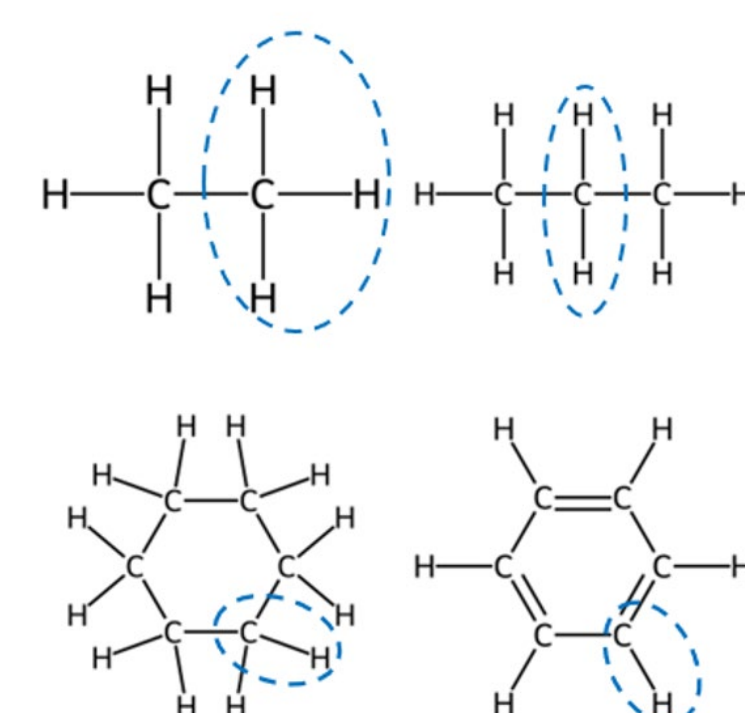
- Incorporate a variety of testing data beyond composition-property test reports
- Apply advanced analysis technique: Machine-Learning based strategies to rapidly generate models and understand uncertainty

### Leverage data to accelerate model development and evaluate novel jet fuel

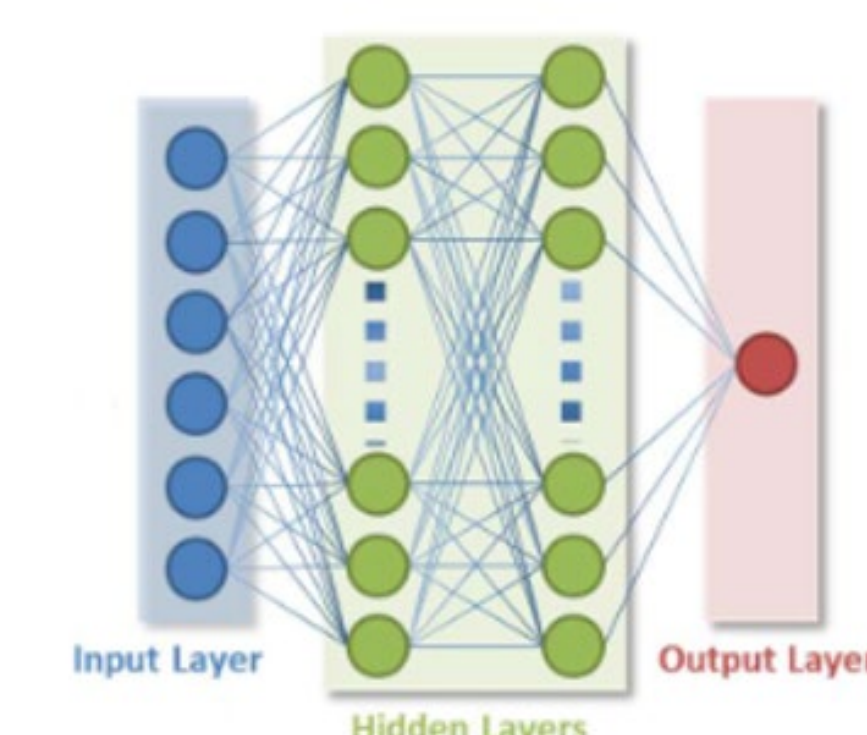
Fuel composition and property data



Fuel Surrogate Modelling with functional groups: Robust approach for novel fuels



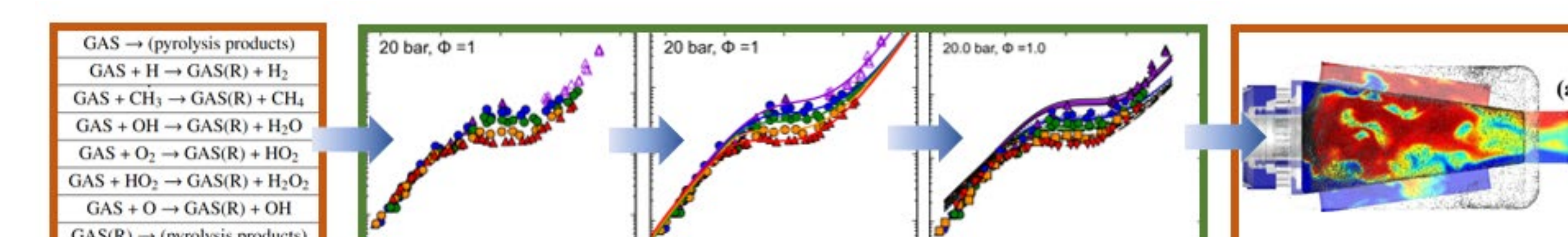
Data Driven Neural Network



Accuracy on par with detailed kinetic simulations with greatly reduced computational time

Rapidly generated kinetic mechanisms for full engine simulations

reactions:  
- equation: SURBLEND  $\Rightarrow$  0.2962668 C<sub>2</sub>H<sub>4</sub> + 1.266519 C<sub>3</sub>H<sub>6</sub> + 0.  
rate-constant: (A: 2.83e+26, b: -2.58, Ea: 8.0197e+04)  
- equation: SURBLEND + H  $\Rightarrow$  H<sub>2</sub> + IC13H27 # Reaction 2  
rate-constant: (A: 8.72e+05, b: 2.4, Ea: 2580.0)  
- eq reactions:  
- eq equation: SURBLEND  $\Rightarrow$  0.2962668 C<sub>2</sub>H<sub>4</sub> + 1.266519 C<sub>3</sub>H<sub>6</sub> + 0.  
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- eq equation: SURBLEND + H  $\Rightarrow$  H<sub>2</sub> + IC13H27 # Reaction 2  
rate-constant: (A: 8.72e+05, b: 2.4, Ea: 2580.0)  
- eq equation: SURBLEND + C<sub>2</sub>H<sub>6</sub>  $\Rightarrow$  C<sub>2</sub>H<sub>4</sub> + IC13H27 # Reaction 3  
rate-constant: (A: 4.64, b: 3.46, Ea: 4600.0)  
- eq equation: SURBLEND + OH  $\Rightarrow$  H<sub>2</sub>O + IC13H27 # Reaction 4  
rate-constant: (A: 4.88e+18, b: 0.51, Ea: 64.0)  
- eq equation: SURBLEND + O<sub>2</sub>  $\Rightarrow$  H<sub>2</sub>O<sub>2</sub> + IC13H27 # Reaction 5  
rate-constant: (A: 1.49e+15, b: 0.0, Ea: 4.3e+04)  
- equation: SURBLEND + H<sub>2</sub>O<sub>2</sub>  $\Rightarrow$  H<sub>2</sub>O + IC13H27 # Reaction 6  
rate-constant: (A: 9830.0, b: 2.77, Ea: 1.05e+04)  
- equation: SURBLEND + O  $\Rightarrow$  OH + IC13H27 # Reaction 7  
rate-constant: (A: 7.85e+04, b: 2.5, Ea: 1110.0)



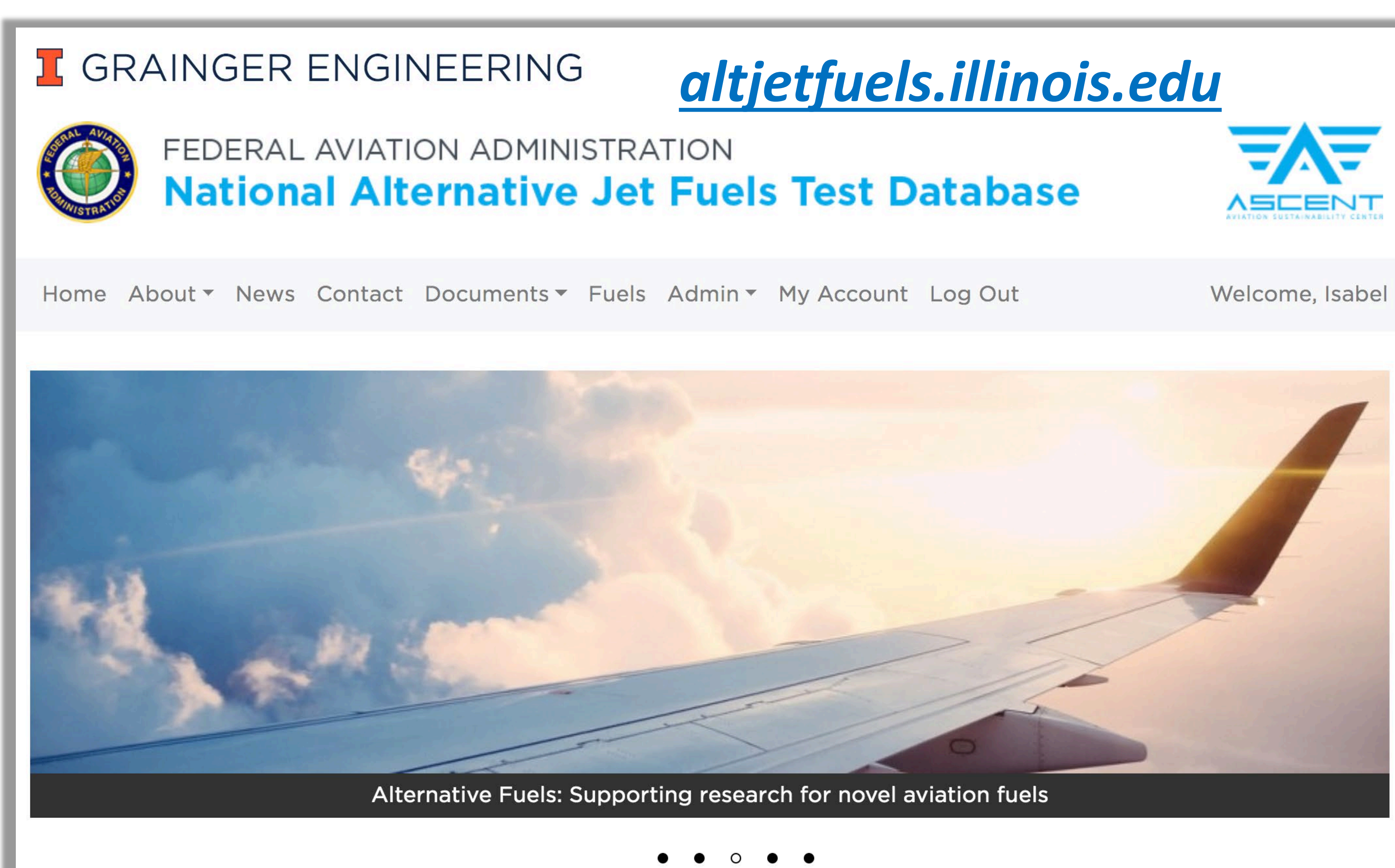
## Conclusions and Next Steps

### Domestic and International Data Sharing:

- Expand scope of airport data collection
  - NY Port Authority
  - HNL
- Implement data pipeline using data format conversion script and create a defined process for new data uploads

### Chemical Kinetics Development:

- Rapid chemical kinetic mechanism generation for any fuel
- Uncertainty Quantification and Reduction



## Research Partners



**NIST** **Ansys** **Honeywell**

**Rolls-Royce** **Williams International**

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Project manager: Ana Gabrielian, FAA

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