ASCENT Project 25

Rapid IR Fuel Screening

(Shock Tube and Flow Reactor Studies of the Kinetics of Jet Fuels)

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Objective:

Develop a **compact, low-volume prescreening tool** for the prediction of physical and chemical properties of sustainable aviation fuels (SAFs) using Fourier-Transform Infrared (FTIR) spectrometry and advanced statistical analysis methods.

Project Benefits:

- FTIR prescreening approach will **make SAF design and approval process less costly and more efficient**.
- This low-volume (<1 mL) method yields insights that are **complementary to other prescreening approaches** (e.g., GCxGC).

Research Approach:

Develop statistical models that **correlate the physical and chemical properties of a fuel** (e.g., boiling point, heat of combustion, flash point, etc.) **with its vapor-phase FTIR spectrum**.

Apply these models to **predict the physical and chemical properties of next-generation SAFs** and fuel components.

Major Accomplishments (to date):

- **Employed blending rules to extend the training dataset** by adding the FTIR spectra and property data of neat hydrocarbon mixtures
- **Trained models for key physical and chemical properties** using the expanded dataset
- The **models successfully predict the properties of all fuels** in the training dataset

Future Work / Schedule:

- **Develop nonlinear regression strategies** to improve predictions of properties with nonlinear dependence on composition
- Optimize models and begin utilization to **predict the properties of SAFs** and SAF components
- Compare IR approach with alternate prescreening methods

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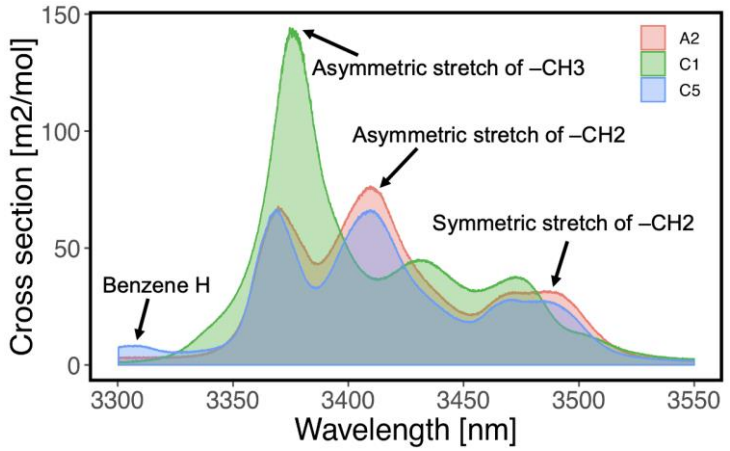
Introduction

Motivation:

- The vapor-phase IR absorption spectrum of a hydrocarbon fuel contains quantitative information about the fuel's molecular structure and functional groups
- Statistical models can be used to infer the physical and chemical properties of fuels from this spectral information

Fuel structure is evident in the IR spectra; shape and height of absorption features reflects the type and number of functional groups, and can be **correlated with physical/chemical properties**



Approach:

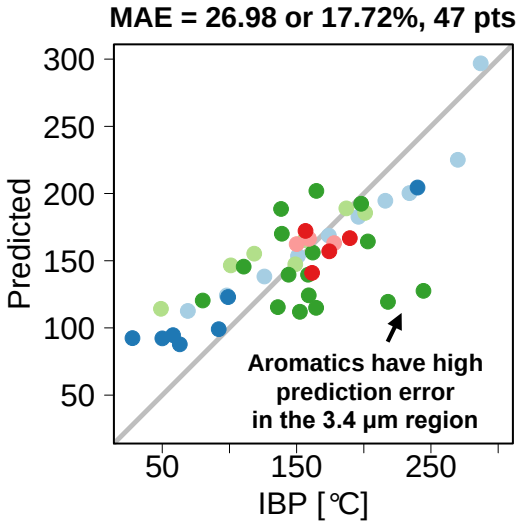
- Develop a training dataset based on broad (2-15 μm) vapor-phase spectra of fuels and their key physical and chemical properties
- Build statistical models using the training data to directly correlate fuel properties, functional groups, and composition with FTIR spectral features
- Use the optimized models to predict the physical and chemical properties of next-generation SAFs and SAF components

FTIR Spectrum [2-15 μm] → **Regularized Linear Models** → **Properties**

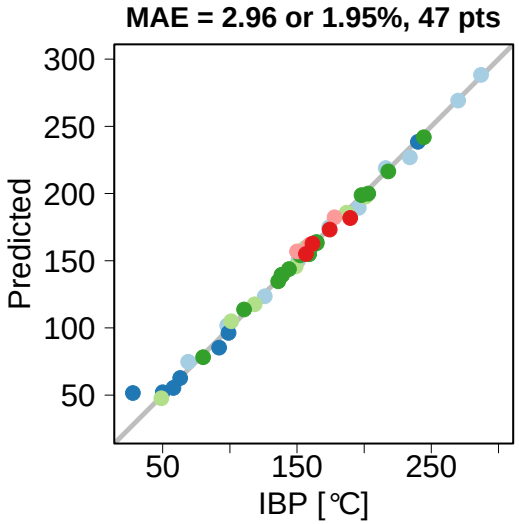
Previously

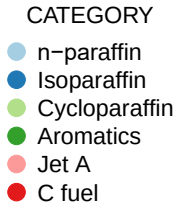
- Introduced the benefits of utilizing the extended 2-15 μm spectral range vs. 3.4-μm region only
- Demonstrated improved model performance for expanded training dataset, which incorporated extended 2-15 μm spectra for real fuels (measured in-house)

Earlier Model
3.4 μm region (N = 24, α = 1)



Current Model
2-15 μm region (N = 496, α = 0.9)





Training cross-validation error

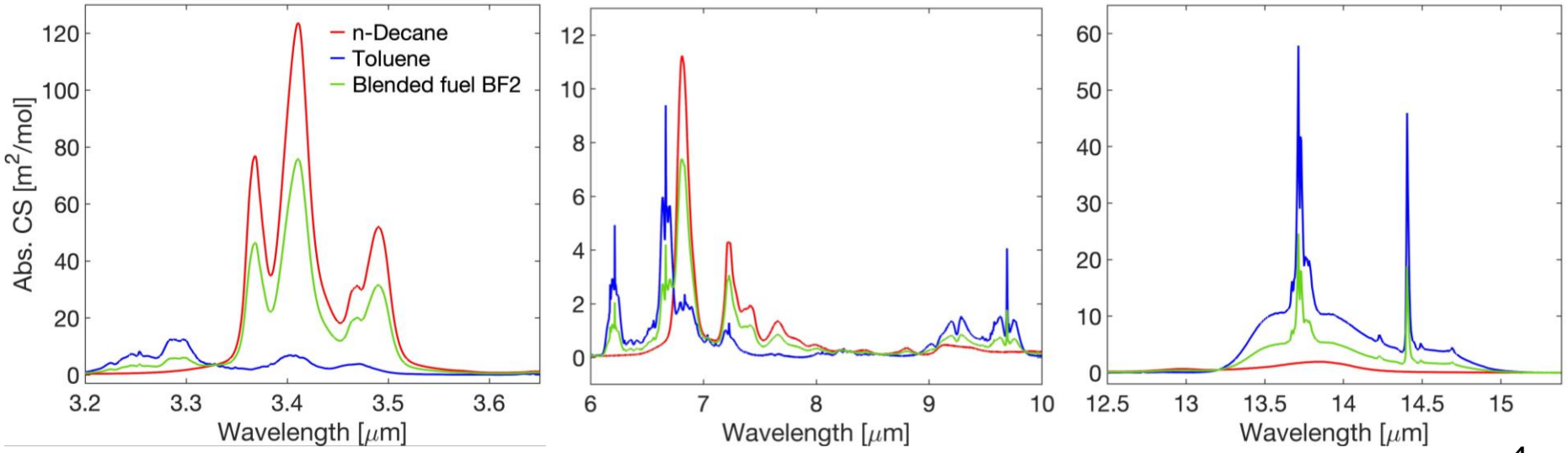
Spectral region	CVE [℃]	CVE (%)	R^2 value
3.4 μm	28.82	18.93%	0.59
2-16 μm	8.55	5.61%	0.99

- **Research question:** Can the training dataset be further expanded by adding simulated spectra?

Further extension of the training dataset using blending rules

- Gas-phase FTIR spectra have a **linear dependence on fuel composition**, offering the ability to calculate a "blended fuel" spectrum as a weighted sum of the spectra of multiple neat components
- The "blending" of the IR spectra of neat hydrocarbons enables the extension of the training dataset **without the need for additional FTIR measurements**
- Calculated spectra of 24 blends of neat hydrocarbons (2-3 components) have now been added to the training dataset
  - Blends composed of n-dodecane, n-decane, isooctane, and toluene

Spectrum of the blended fuel BF2: 59.2% n-Decane + 40.8% Toluene



Blending rules for property data

- Blending rules were used to calculate net heat of combustion (NHC), threshold sooting index (TSI), and kinematic viscosity (KV) property values for the 24 neat hydrocarbon mixtures
- The number of data points available for each property in the training dataset, after applying the blending correlations, is shown below:

Property	Number of fuels		Type of blending rule
	Previous dataset	Expanded dataset	
NHC	35	59	Linear
TSI	20	44	Linear
KV	31	55	Non-linear

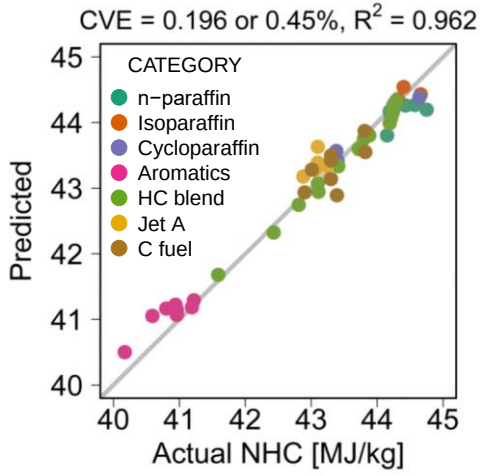
- The **larger sample size of the expanded dataset is expected to improve the prediction accuracy** of the regularized linear models for all three properties

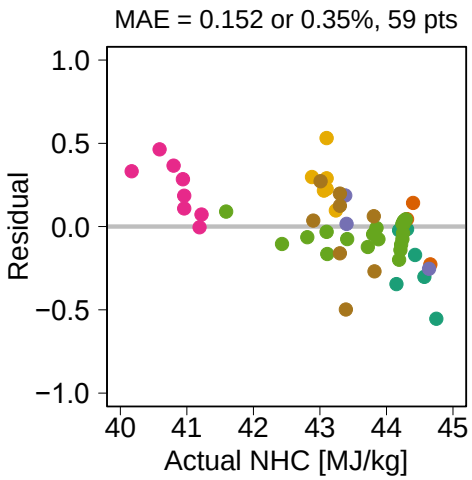
Model Performance for NHC and TSI

- Regularized linear models were trained on the expanded dataset for **net heat of combustion (NHC)** and **threshold sooting index (TSI)**

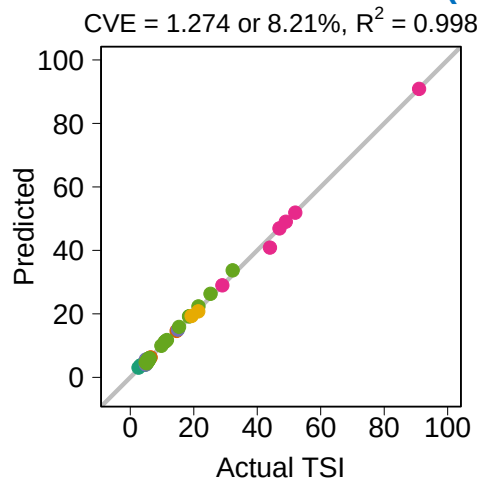
- The models show **high prediction accuracy** for both properties, as evidenced by the **low mean absolute error (MAE) of prediction** on the training data
- The **high R^2 values** indicate that both the models fit the training data well, and the **low cross-validation error (CVE)** highlights the potential of this approach for making highly accurate future property predictions
- Since the blending rules used for these properties are linear, **the regularized linear models accurately estimate the properties of the hydrocarbon blends**

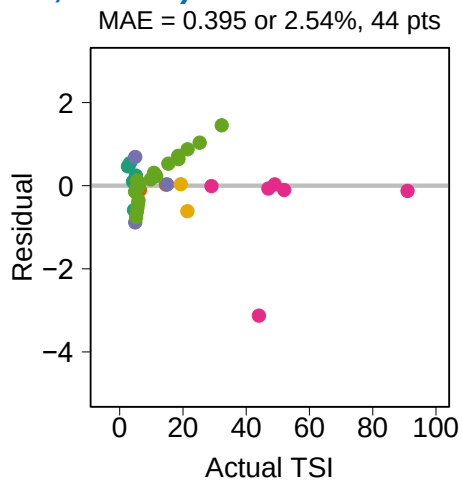
NHC Model (N = 208, α = 0.3)





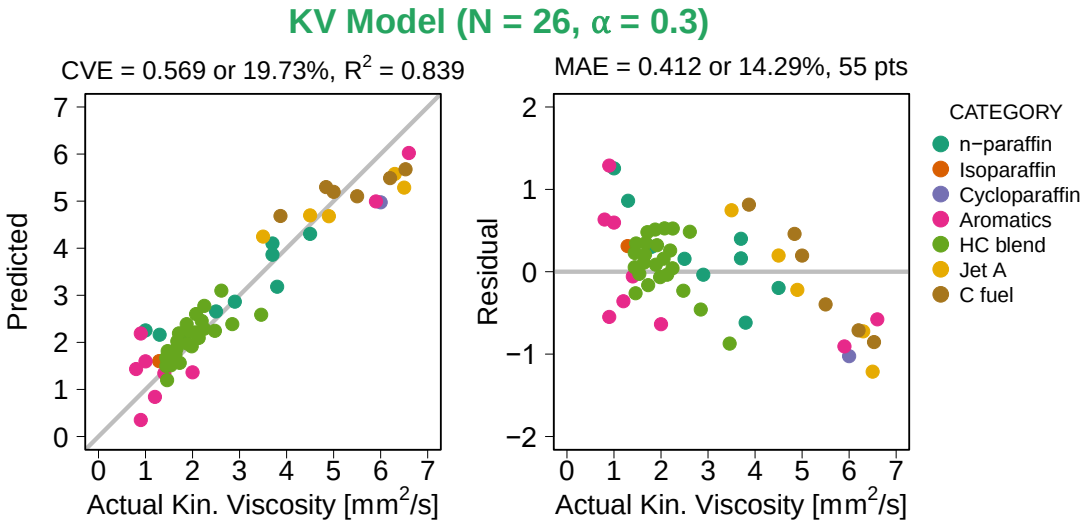
TSI Model (N = 32, α = 0.1)





Model Performance for KV

- A regularized linear model was also developed for the property **kinematic viscosity (KV)** - a property with non-linear dependence on composition



- Although the model fits the training data reasonably well, the **predictive accuracy is not as high** as in the case of NHC and TSI
- This is indicated by the **higher CVE and MAE**, and the **lower R^2** value compared to the other properties
- The blending rule employed for KV clearly shows that **viscosity exhibits a strongly non-linear dependence on fuel composition**, thus suggesting the need for a revised modeling approach for some properties

Summary and Future Work

- IR spectral analysis offers a **robust, low-volume way to predict the physical and chemical properties of fuels**
- **Blending rules were used to calculate the FTIR spectra and properties of neat hydrocarbon mixtures** to expand the training dataset
- Regularized linear models trained on the expanded training dataset show **excellent predictive performance for NHC and TSI**, with scope for further improvement in the case of KV

Next steps:

- **Develop nonlinear regression strategies** to improve the prediction accuracy for highly nonlinear properties like kinematic viscosity
- Continue optimization of models, use them to **predict the properties of SAFs** and SAF components, and compare model performance with alternate methods
- Increase ASCENT collaboration (P65): investigate the **impact of isomeric structure on key properties** such as ignition delay time (IDT) and freezing point