ASCENT Project 25

Rapid IR Fuel Screening

(Previously: 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):

- Separate **models have been trained for key physical/chemical properties** using a dataset of pure hydrocarbons
- The **models accurately predict the properties of all fuels** in the training dataset
- An FTIR spectrometer facility has been modified to enable wide-spectrum IR measurements (2-16 μm)

Future Work / Schedule:

- Expand the training dataset to include more fuels (>C8) and additional property data
- Use the optimized models to predict the properties of SAFs and SAF components
- Explore other prescreening opportunities enabled by IR spectral analysis

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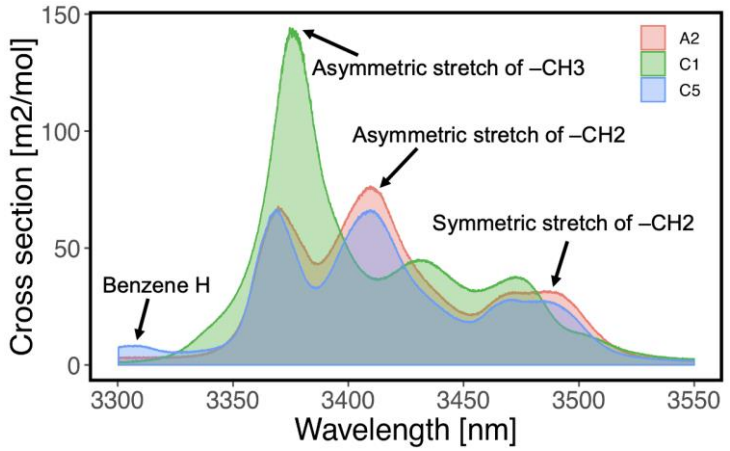
Introduction

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:

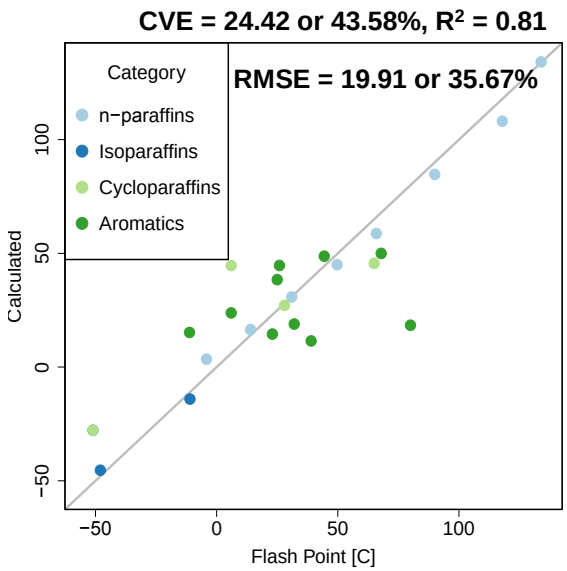
- Develop a training dataset containing the vapor-phase Fourier-Transform Infrared (FTIR) spectra (2-16 μm) of fuels and their key physical and chemical properties
- Build statistical models using the training data to directly correlate fuel properties with their FTIR spectra; four different models under consideration
- Use the optimized models to predict the physical and chemical properties of next-generation SAFs and SAF components

FTIR Spectrum [2-16 μm] → **Model 1: Regularized Linear Model** → **Properties**

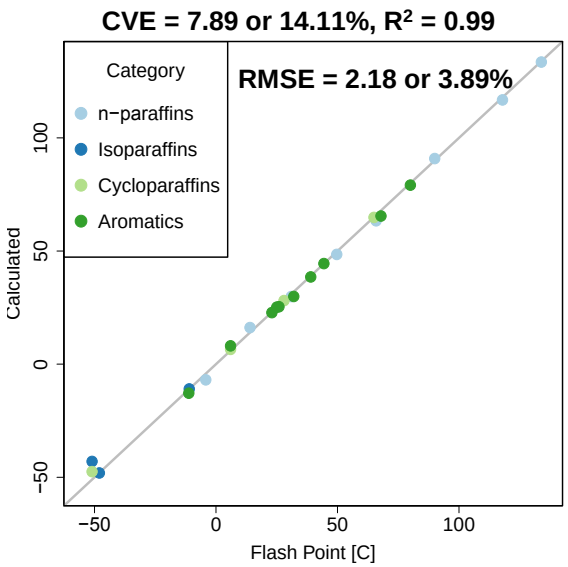
Recent Progress and Results

Benefits of the extended spectral range: Flash Point (℃) prediction

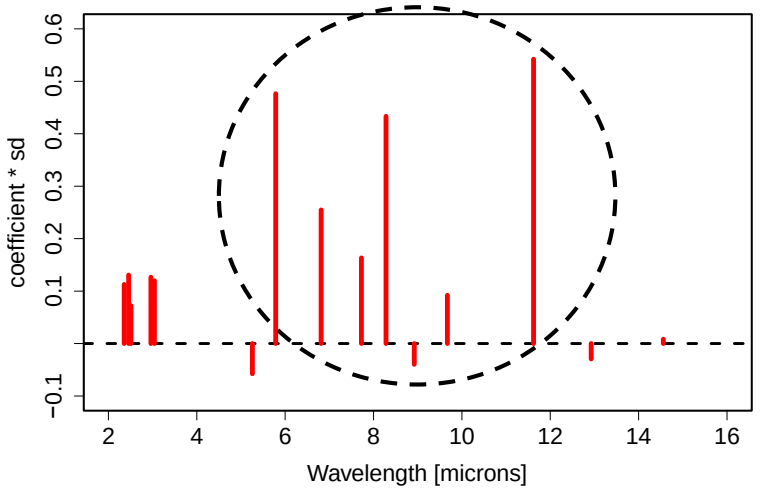
3 μm region only



2-16 μm region



Relative contribution of selected wavelengths



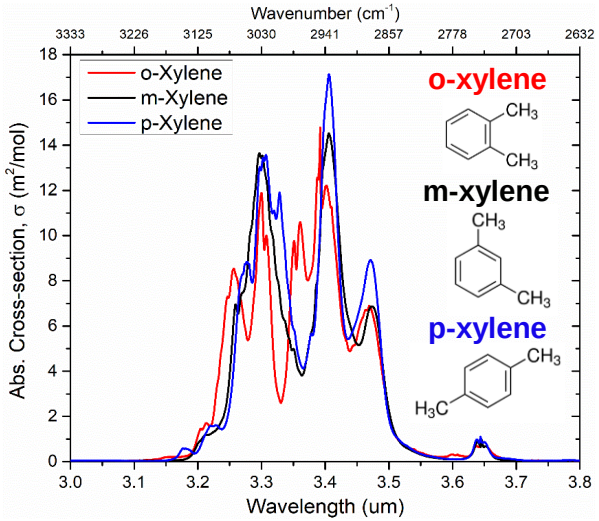
- The regularized linear model is **optimized separately for each target property**, using a training dataset currently limited to pure hydrocarbons
- Using the **full 2-16 μm region greatly improves the prediction accuracy** due to the relatively large contribution of wavelengths outside the 3 μm region to the variation in flash point
- The high R^2 value indicates that the model fits the training data well, and the low cross-validation error (CVE) highlights the potential of this approach for making **highly accurate future property predictions**

IR spectral analysis as a complementary approach to GC

Isomeric distinction:

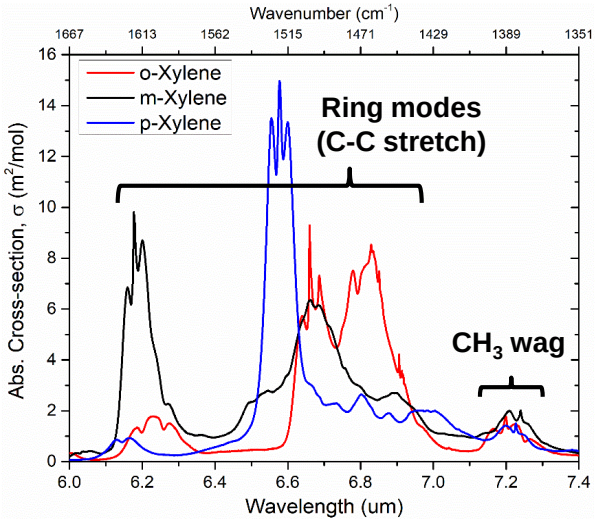
- Certain physical **properties** (e.g., freezing point) **vary significantly** among the **different structural isomers** of a molecule
- IR spectra (2-16 μm) are highly sensitive to the molecular structure, and hence can be used to **detect differences between structural isomers**

Example: The Three Isomers of Xylene (Dimethylbenzene)



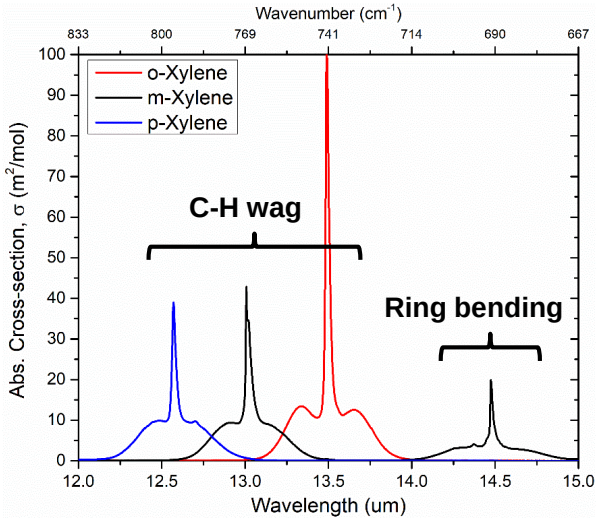
3-4 μm region

Isomeric distinction: **Difficult**



6-7 μm region

Isomeric distinction: **Possible**



12-15 μm region

Isomeric distinction: **Yes**

- IR spectral analysis therefore **supplements the GCxGC approach**, which is limited in its ability to distinguish between isomers

Summary and Future Work

- IR spectral analysis offers a **robust, low-volume way to predict the physical and chemical properties of fuels**
- Regularized linear models trained on a dataset of pure hydrocarbons showed **excellent predictive performance for all the properties considered**
- This approach can be used to effectively distinguish between isomers, thus providing a **complementary approach to GC-based fuel analysis methods**

Next steps:

- Expand the current training dataset to include more pure hydrocarbons (larger than C8) and real fuels using new measurement capability of our in-house FTIR
- Use the optimized models to predict the properties of SAFs and SAF components
- Assess the ability of the developed models to accurately infer the relevant structural isomer components
- Develop strategies to identify the molecular composition of blended fuel mixtures using IR spectra and evaluate the effect of fuel additives on mixture properties
- Explore the potential for predicting rig testing performance and fundamental combustion properties of fuels using IR spectral analysis (IR-HyChem)