ASCENT Project 25

Rapid IR Fuel Screening

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

Stanford University
PI: Ronald K. Hanson
PM: Anna Oldani
Cost Share Partner: Stanford University

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):

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

Future Work / Schedule:

- **Continue expanding the training dataset** to include more fuels (>C8) and additional property data
- Optimize models and begin utilization to **predict the properties of SAFs** and SAF components
- Compare IR analysis approach with alternate prescreening methods

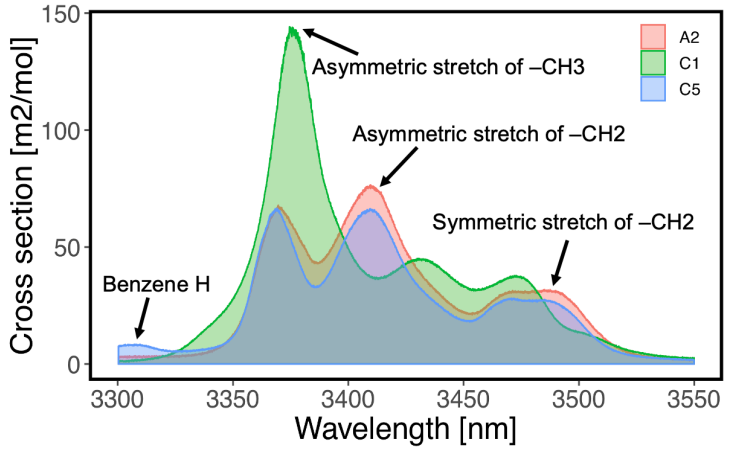
This research was funded by the U.S. Federal Aviation Administration Office of Environment and Energy through ASCENT, the FAA Center of Excellence for Alternative Jet Fuels and the Environment, project 25 through FAA Award Number 13-C-AJFE-SU-017 under the supervision of Anna Oldani. Any opinions, findings, conclusions or recommendations expressed in this this material are those of the authors and do not necessarily reflect the views of the FAA.

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 (2-16 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 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**

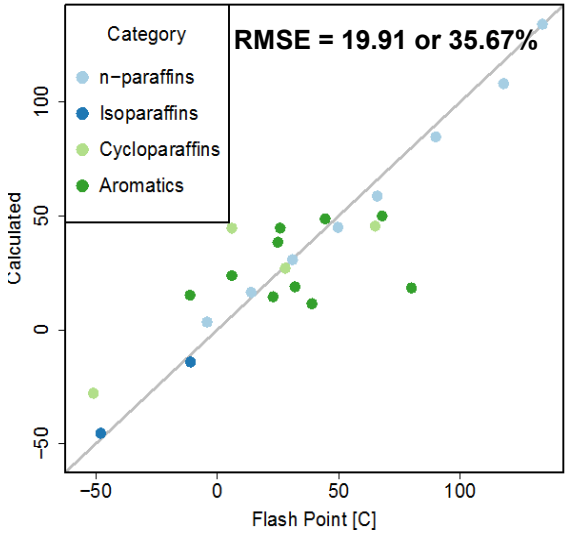
Previously

- Introduced the benefits of utilizing the extended 2-16 µm spectral range vs. 3.4-µm region only

Property prediction example: Flash Point (℃)

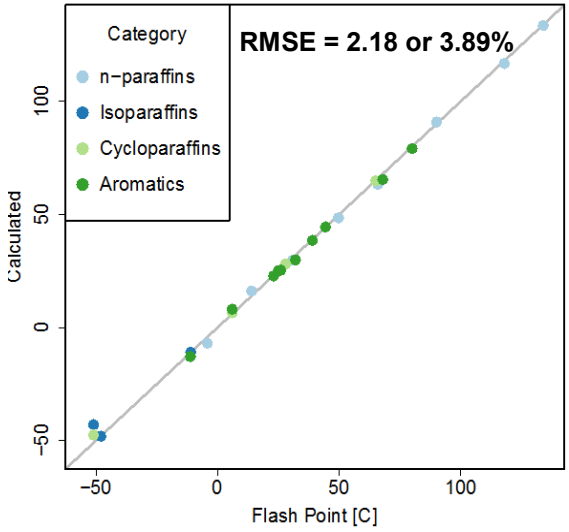
3.4 µm region only

CVE = 24.42 or 43.58%, R^2 = 0.81

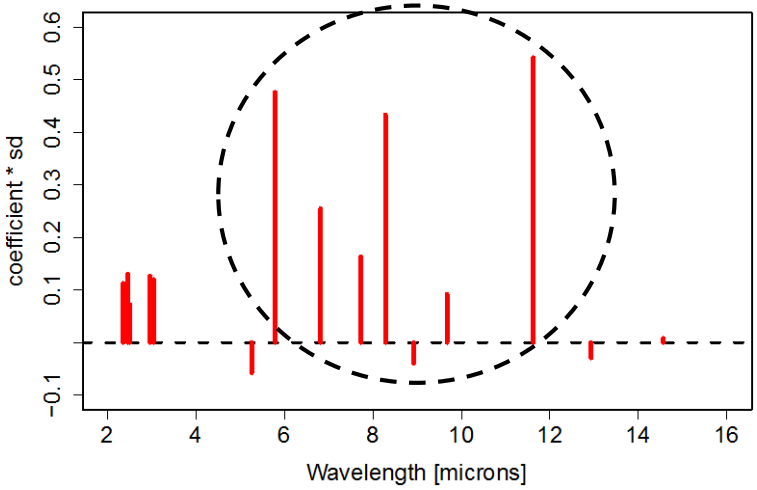


2-16 µm region

CVE = 7.89 or 14.11%, R^2 = 0.99



Relative contribution of selected wavelengths



- Previous wide-spectrum analysis relied exclusively on spectra available in public Pacific Northwest National Lab (PNNL) database
- **Research need:** measurement of the 2-16 µm spectra of **real fuels and pure hydrocarbons** not included in the PNNL database

Recent Progress

- The **FTIR experimental setup was modified** to enable measurement of gas-phase fuel spectra across the full 2-16 μm region
  - Heated-cell windows replaced to enable wide-spectrum transmission, purge system constructed

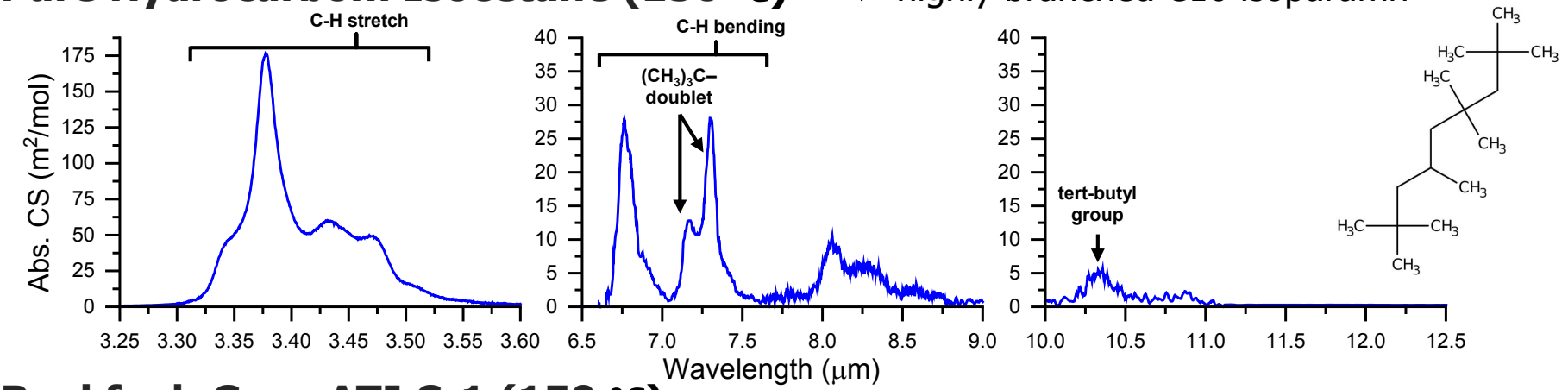
- Stanford has now measured 15 pure hydrocarbons and real fuels, expanding our 2-16 μm training dataset to 71 fuels:

Fuel category	Stanford-Measured Spectra	PNNL Spectra	
n-paraffins	2	8	C5-C16 neat hydrocarbons
Isoparaffins	2	5	
Cycloparaffins	3	4	
Aromatics	1	15	
Multi-comp. blends	0	24*	
Real fuels	7	0	
Total	15	56	71 Fuels

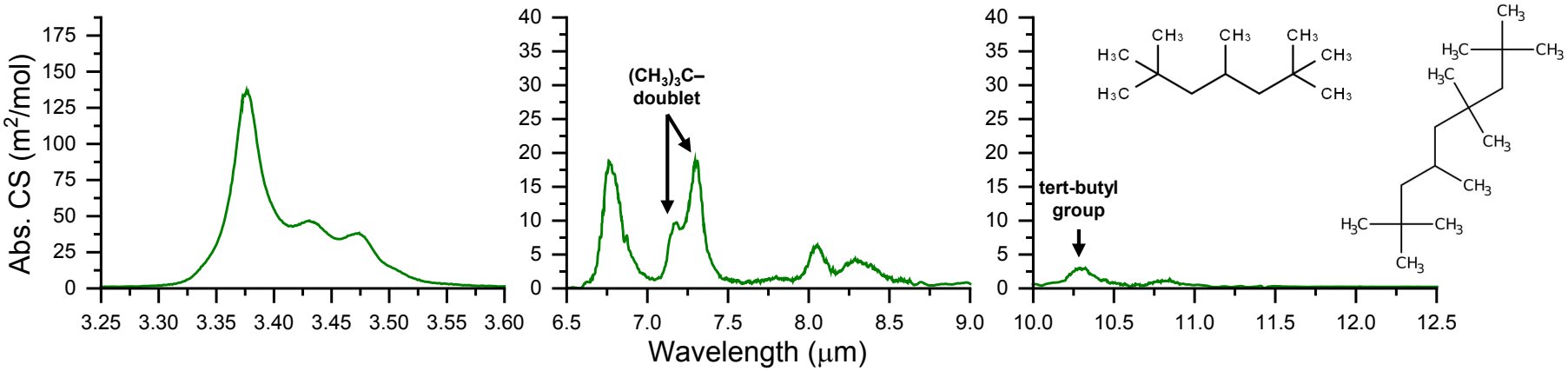
*weighted combination of individual components

Example of Newly Measured Spectra

Pure Hydrocarbon: Isocetane (150 ℃) → highly branched C16 isoparaffin



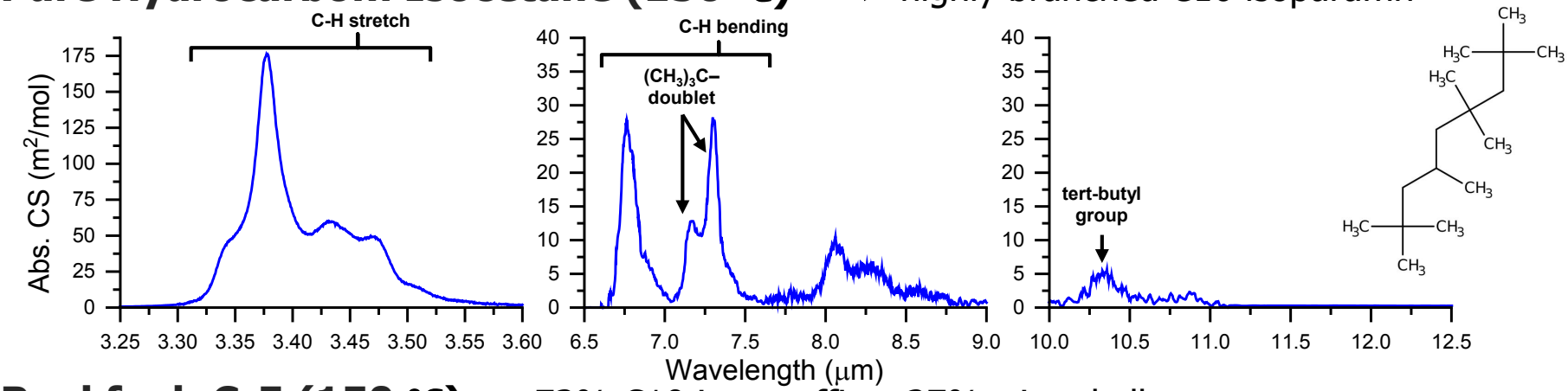
Real fuel: Gevo ATJ C-1 (150 ℃) → predominantly isocetane, 2,2,4,6,6-pentamethylheptane



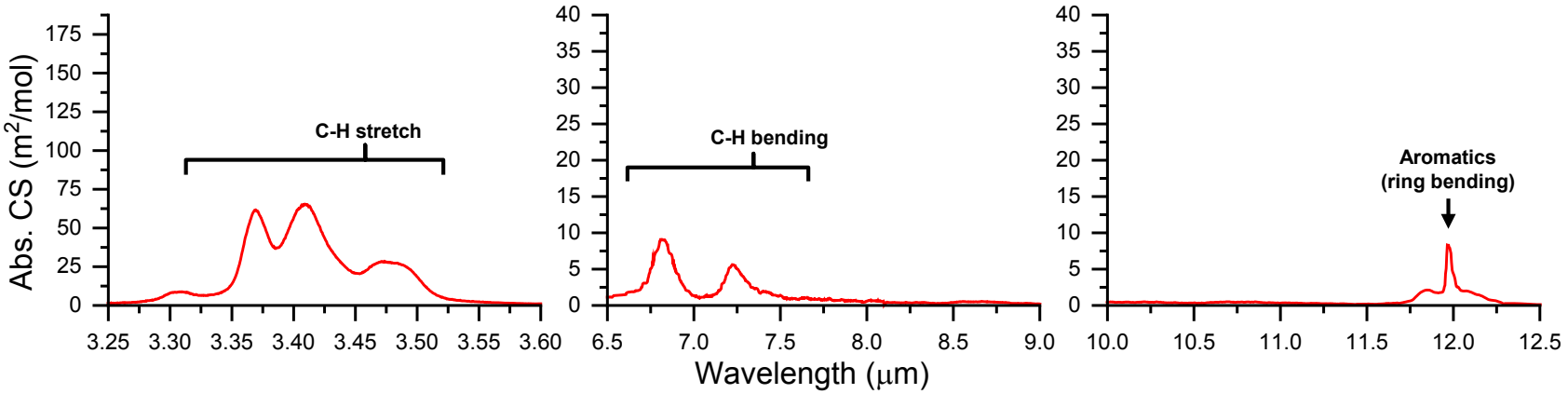
- Using multiple fuel concentrations enables **good signal-to-noise ratio** across the entire 2-16 μm range
- As expected, prominent **features seen in the isocetane spectrum also appear in the C-1 spectrum**

Example of Newly Measured Spectra

Pure Hydrocarbon: Isocetane (150 ℃) → highly branched C16 isoparaffin



Real fuel: C-5 (150 ℃) →73% C10 isoparaffins, 27% trimethylbenzene

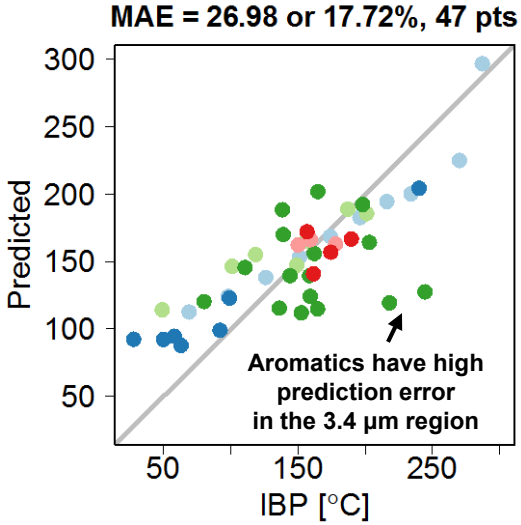


- Using multiple fuel concentrations enables **good signal-to-noise ratio** across the entire 2-16 μm range
- **Clear differences observed between the isocetane and C-5 spectra** (shape, height, location of spectral features)

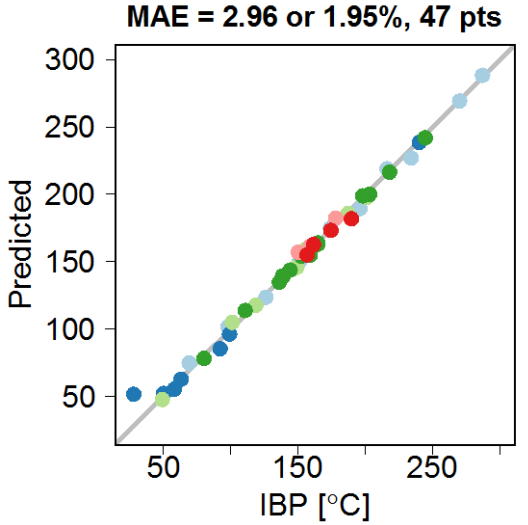
Model Performance (2-16 µm)

- The prediction accuracy of the previous 3.4 µm model and the new 2-16 µm model are compared for **initial boiling point (IBP)**

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



Current Model
2-16 µm region (N = 496, α = 0.9)



Training cross-validation error

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

- Using the expanded training dataset and 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 IBP
- 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**

Summary and Future Work

- IR spectral analysis offers a **robust, low-volume way to predict the physical and chemical properties of fuels**
- Modification of our FTIR spectrometer setup has **enabled measurement of gas-phase, 2-16 µm spectra** of relevant hydrocarbon fuels and SAFs
- Regularized linear models trained on the expanded training dataset show **excellent predictive performance for all the properties considered**

Next steps:

- **Continue use of FTIR to expand the current training dataset** to include more pure hydrocarbons (larger than C8) and real fuels
- Continue optimization of models, use them to **predict the properties of SAFs** and SAF components, and compare model performance with alternate methods
- ASCENT collaboration (J. Heyne, U. Dayton): investigate the **impact of isomeric structure on ignition properties**