Project 025 Shock Tube Studies of the Kinetics of Jet Fuels

Stanford University

Project Lead Investigator

Ronald K. Hanson
Woodard Professor
Mechanical Engineering Department
Stanford University
452 Escondido Mall
650-723-6850
rkhanson@stanford.edu

University Participants

Stanford University

- P.I.: Prof. Ronald K. Hanson
- FAA Award Number: 13-C-AJFE-SU-027
- Period of Performance: October 1, 2024, to September 30, 2025
- Task:
  1. Chemical kinetics combustion experiments.

Project Funding Level

In 2024–2025, the Federal Aviation Administration (FAA) provided $400,000 in funding and Stanford University provided $400,000 in 1:1 matching funds.

Investigation Team

Prof. Ronald K. Hanson, P.I., research direction
Jesse W. Streicher, Research Scientist, research management
Miguel Figueroa Labastida, Postdoctoral fellow, research assistance
Andrew R. Klingberg, Graduate Student, research assistance

Project Overview

This year’s efforts focused on advancing Fourier transform infrared (FTIR)-based tools for rapid fuel prescreening by integrating compositional inference, thermochemical property estimation, and comparative modeling analysis. First, we extended our spectral-surrogate framework to predict key thermochemical properties, demonstrating that molecular-species information inferred from vapor-phase mid-infrared (IR) spectra can be used to accurately estimate specific heat, enthalpy, and entropy. Second, we evaluated the generality of an existing molecular-weight prediction model by testing it against a new set of World Jet Fuel Survey (WJFS) samples. Additionally, we developed an improved model tailored to this fuel population. Finally, we systematically compared three representations of the FTIR spectrum, including raw cross-section data, Principal component analysis (PCA)-reduced features, and spectral moments, to quantify their impacts on predictive accuracy, reproducibility, and model development complexity. Together, these studies refine the methodological foundation needed for spectrum-based characterization of aviation fuels and support the development of reliable, data-driven prescreening tools for emerging fuel candidates. In parallel, an instrumentation upgrade to the Thermo Fisher Scientific® Nicolet™ iS50 FTIR system expanded our measurement capabilities and will further enhance future model development.

® Thermo Fisher Scientific and Nicolet are registered trademarks of Thermo Fisher Scientific, Inc., Waltham, Massachusetts.

Task 1 – Chemical Kinetics Combustion Experiments

Stanford University

Objectives

This work is aimed at developing fuel prescreening tools based on the IR absorption cross-section measurements of jet fuels and their constituent molecules. Specific fuel analysis objectives include developing effective strategies for correlating (a) chemical, physical, and combustion properties, and (b) functional group and molecular species composition of jet fuels with their IR spectra.

Research Approach

An important goal of the current research is to characterize jet fuel composition and properties based on the fuel's mid-IR absorption spectrum, measured using a FTIR spectrometer. Over the past five years, a database of spectroscopic measurements and property data for a variety of jet fuels and jet fuel components has been collected. Using this database, we have developed linear and nonlinear correlations between the spectroscopic properties of jet fuels with fuel composition and with important physical/chemical properties such as density, derived cetane number, net heat of combustion, and flash point. Here, we present an overview of this year's research areas: using compositional inference to predict thermochemical properties, refining a property prediction model for WJFS fuels, and evaluating how alternative FTIR spectral representations (raw spectra, PCA-reduced data, and spectral moments) impact model accuracy.

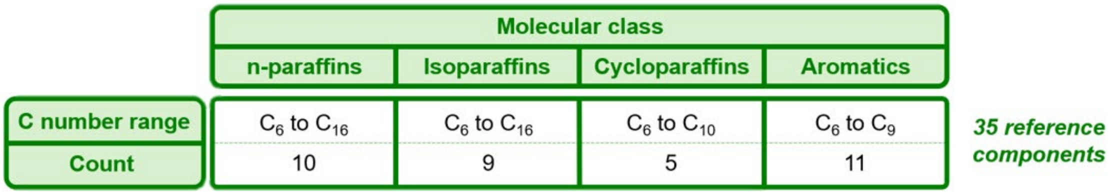
Thermochemical Property Prediction

Traditional approaches for estimating thermochemical properties of real jet fuels rely on constructing a simplified surrogate mixture that approximates the bulk fuel. Because real fuels contain hundreds of molecular species, these surrogates are typically limited to only two to four neat hydrocarbons selected to reproduce a small set of global physical properties (e.g., density, hydrogen-to-carbon ratio, or average carbon number). Once selected, the thermochemical properties of the surrogate are computed as the mole-fraction-weighted sum of the property contributions from each component. While effective for broad characterization, this approach is fundamentally constrained by the limited number of components and by the reliance on global properties, which limits its ability to capture detailed molecular-level features that strongly influence heat capacity, enthalpy, and entropy.

In contrast, an FTIR-based approach (Strategy 4) leverages the rich spectral information contained in vapor-phase mid-IR measurements to inform surrogate formulation. Instead of constraining the surrogate to just a few components, we begin by measuring the vapor-phase FTIR spectrum of the real fuel and then identify the mixture of neat-component spectra that best reconstructs the measured spectrum. Because vapor-phase absorption cross sections are linearly additive, the reconstructed "spectral surrogate" is not restricted in component count and can incorporate contributions from a broad set of reference molecules. This year, we expanded and utilized a reference library containing vapor-phase spectra and thermochemical data for 35 hydrocarbons, spanning paraffins, isoparaffins, cycloalkanes, and aromatics. Both the spectrum and the thermochemical properties of these components are linearly additive, enabling consistent mapping between spectral fit and thermochemical prediction.

Table 1 provides an overview of the neat-component reference library. By leveraging this library and the spectral additivity principle, Strategy 4 allows the surrogate mixture to more accurately reproduce the molecular structure of the target fuel, which in turn yields accurate predictions of specific heat, enthalpy, and entropy.

Table 1. Overview of reference library of neat components. The library includes vapor-phase spectra and thermochemical data for 35 hydrocarbons.



	Molecular class			
	n-paraffins	Isoparaffins	Cycloparaffins	Aromatics
C number range	C_6 to C_{16}	C_6 to C_{16}	C_6 to C_{10}	C_6 to C_9
Count	10	9	5	11

35 reference components

To obtain the spectral surrogate, a constrained linear least-squares optimization is used to determine the mole fractions of the neat components. The optimization enforces non-negativity of all component fractions, ensures that the mixture fractions sum to unity, and matches the average carbon and hydrogen numbers of the target fuel. Using these constraints, the solver identifies the combination of reference spectra that best reproduces the measured vapor-phase FTIR spectrum of Jet-A fuel. The resulting surrogate mixture captures the major spectral features of the fuel, with remaining differences primarily arising from gaps in the reference library; these discrepancies can be further reduced by expanding the set of available neat-component spectra. Figure 1 presents a comparison between the measured Jet-A (A2) spectrum and Strategy-4-derived spectral reconstruction, illustrating the close match achieved by the surrogate.

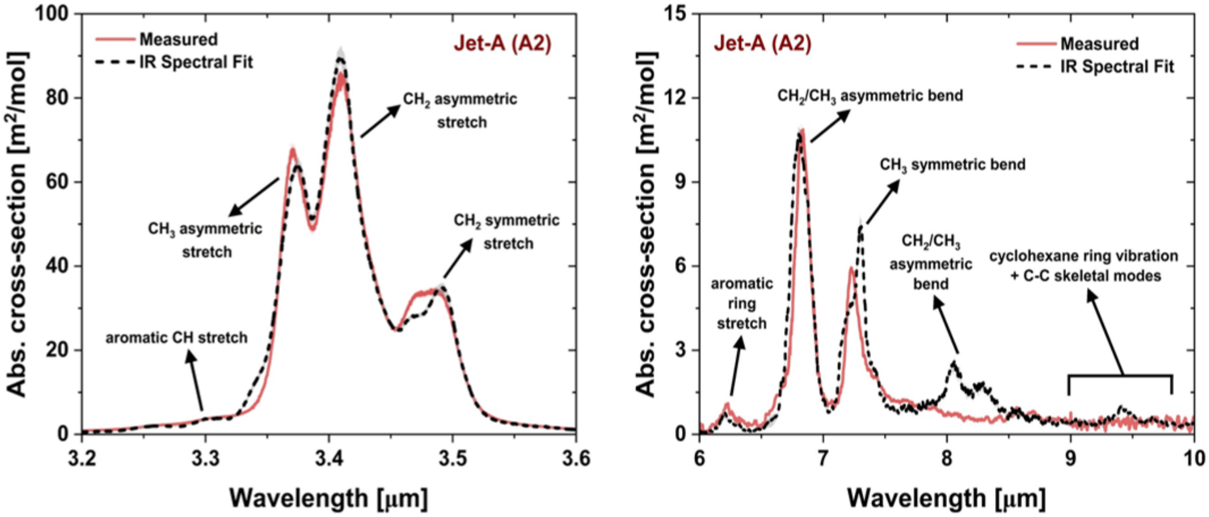


Figure 1. Comparison of measured Jet-A spectrum and the spectrum obtained from Strategy 4.

The thermochemical properties of the surrogate were obtained using National Aeronautics and Space Administration (NASA) polynomial fits for each neat component, which provide temperature-dependent values of specific heat (Cp), enthalpy (H), and entropy (S). Using the mole fractions determined by the spectral fitting procedure, the Cp, H, and S of Jet-A fuel were calculated as linear combinations of the component contributions across a range of temperatures. The resulting estimates agree well with values reported from established Jet-A surrogate models (Figure 2), demonstrating the consistency of the spectral-surrogate approach. Minor differences between models are expected due to variations in component selection and reference data, but these discrepancies are small and are not anticipated to significantly influence global combustion predictions.

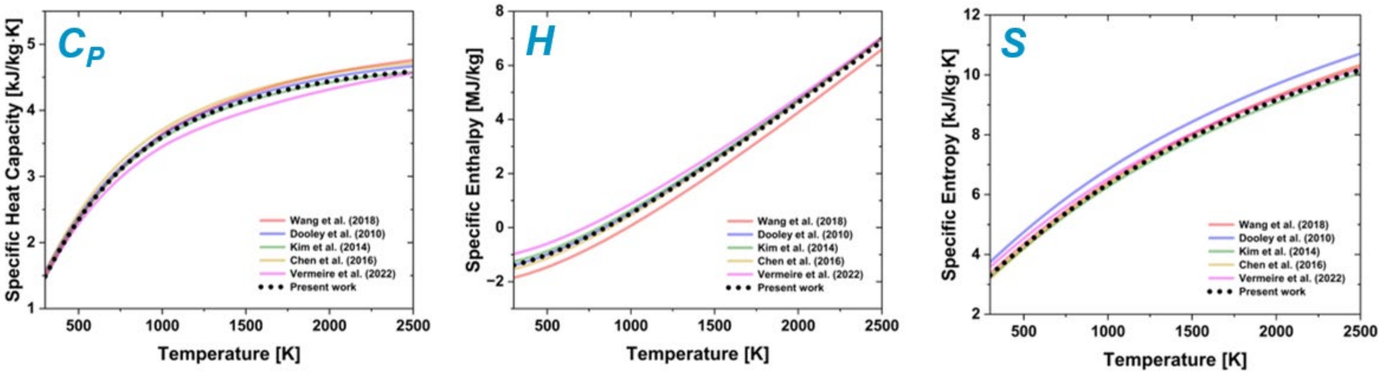


Figure 2. Comparison of specific heat capacity, specific enthalpy, and specific entropy for Jet- predicted from the spectral surrogate (black points) with Jet-A surrogates from the literature.

Adiabatic flame temperature calculations were used as a quantitative metric to assess the performance of the FTIR-based surrogate relative to conventional surrogate formulations. Across a wide range of equivalence ratios, the IR-inferred surrogate (Strategy 4) produces flame temperatures that closely match those obtained from established Jet-A surrogate models (Figure 3), indicating that the spectral surrogate preserves the key thermochemical characteristics governing combustion behavior. Together, these results demonstrate that FTIR measurements, paired with compositional inference, enable accurate prediction of temperature-dependent fuel properties. This approach provides a robust pathway for evaluating the reactivity and combustion performance of novel or emerging fuel candidates during the prescreening process.

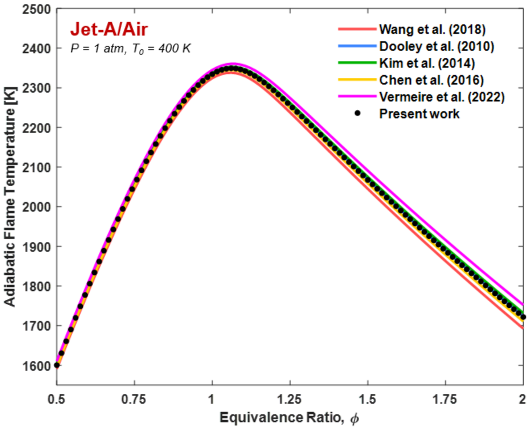


Figure 3. Comparison of simulated adiabatic flame temperature using predicted thermochemical properties from Strategy 4 and Jet-A surrogates from literature.

World Jet Fuel Survey Property Prediction

To evaluate the generality of our existing molecular-weight prediction model, we applied the previously published model of Boddapati et al. (2024) to a new set of WJFS samples. We received 39 WJFS fuels along with property data for 38 of them, and each sample was analyzed using its measured vapor-phase FTIR spectrum. The original model had been trained on a diverse dataset consisting of 47 neat hydrocarbons, 164 simple binary and ternary blends, and 16 jet fuels. When tested on the 38 WJFS samples, however, the model consistently overpredicted molecular weight, indicating that the training set did not fully capture the compositional variability present in the new fuels. This outcome demonstrated the need to further generalize or tailor the existing model for broader fuel classes.

To address this limitation, we developed a new molecular-weight prediction model trained exclusively on the WJFS data. Using 34 samples for training and holding out 4 for testing, the new model produced substantially improved predictive accuracy. This result highlights the importance of selecting a training dataset that closely reflects the fuels of interest, particularly when targeting property prediction for complex real-world mixtures. Figure 4 compares the performance of the original model with the WJFS-trained model and illustrates the improved agreement achieved when the model is calibrated to the specific fuel population. In the improved-model plot (right), blue points mark the samples used for training, and red points denote the held-out test samples that provide an unbiased evaluation of model performance.

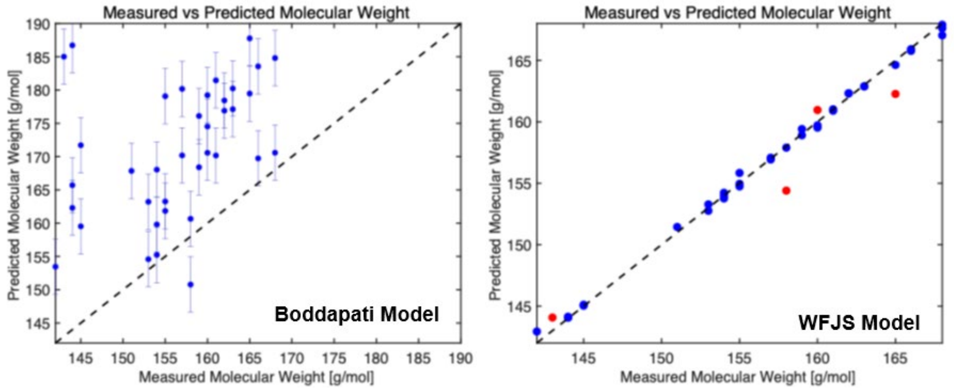


Figure 4. Comparison of molecular-weight prediction performance between the previously developed model and the model trained specifically on WJFS samples.

Model Input Comparison

Our FTIR-based modeling framework was expanded to compare three different spectral input representations: (1) raw vapor-phase FTIR spectra, (2) principal-component–reduced spectra, and (3) spectral-moment descriptors. Using a dataset of 267 fuel spectra, we evaluated how each representation affected both predictive accuracy and model robustness across multiple training subsets. Raw spectra offer the highest physical interpretability (each wavelength corresponds directly to an absorption cross section) but the tens of thousands of input features increase the chance of overfitting and can cause models to select slightly different wavelength regions each time they are retrained. PCA-reduced spectra address this challenge by compressing the data into a small number of orthogonal components that capture the dominant variance in the dataset; however, these components blend many wavelengths and thus are less directly tied to specific functional groups. Spectral moments provide a middle ground: they dramatically reduce the number of features while maintaining physical interpretability. For each predefined functional-group wavelength region, we compute a set of statistical descriptors (including area (zeroth moment), centroid (first moment), width, and skewness) that summarize the shape and strength of the absorption band. Because these features are user-defined rather than model-selected, spectral moments remained consistent across training subsets and offered the highest reproducibility, whereas raw and PCA-based representations provided the strongest predictive accuracy for properties such as molecular weight and density. Table 2 summarizes the three FTIR representations used in model development.

Table 2. Overview of different input representations of the FTIR spectrum used for model development.

Raw Spectrum	Principal Components	Spectral Moments
Physically interpretable: Wavelengths tied to functional groups	**Harder to interpret:** Features are blends of all wavelengths	**Physically interpretable:** Moments tied to functional groups
Large feature set: Tens of thousands → overfitting risk	**Compact feature set:** Captures variance well	**Compact feature set:** Pre-defined and dataset-independent
Stability: Specific wavelengths may change between models	**Stability:** Dependent on dataset composition, but generally consistent	**Stability:** Constant across datasets as the features are determined by user

Figure 5 compares the predictive performance of models trained using the three spectral input representations. For this analysis, all 267 vapor-phase spectra were used to construct the full feature sets for the raw spectrum, PCA-reduced spectrum, and spectral-moment descriptors. A linear regression model was trained for each representation, with hyperparameters optimized through cross-validation. Overall, both the raw-spectrum and PCA-based models achieved the highest accuracy for predicting density, with the raw spectrum slightly outperforming PCA on average. Spectral moments also produced strong predictions but remained the weakest of the three methods in terms of absolute accuracy. These results indicate that when the training dataset adequately represents the fuels of interest, raw or PCA-based inputs are preferred for maximizing predictive performance. Spectral moments remain valuable, however, when stability, reproducibility, or interpretability are the primary objectives.

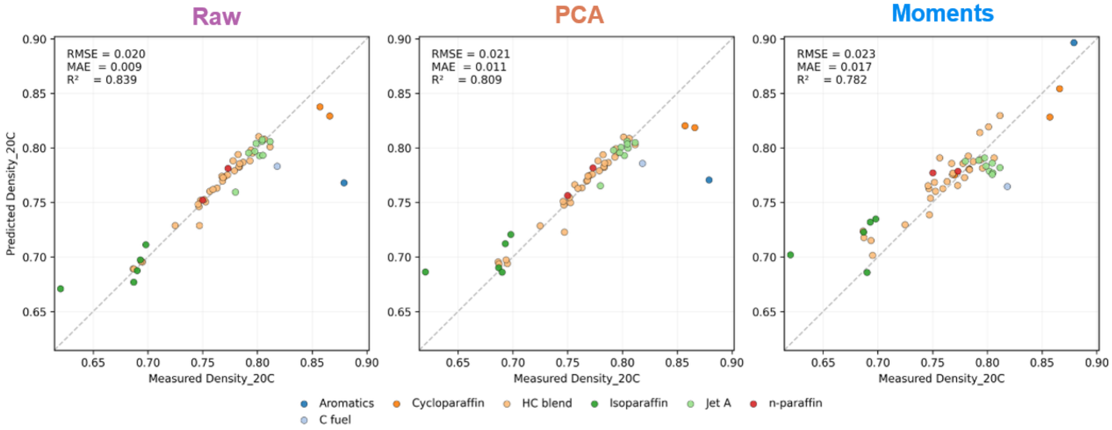


Figure 5. Density property prediction model results using the raw FTIR spectrum, principal components, and spectral moments as the input features for model training.

Instrumentation Update

This year, we acquired a new FTIR spectrometer (Thermo Fisher Scientific Nicolet iS50), which significantly expands our experimental capabilities. The Nicolet iS50 provides an extended spectral range from 1 to 200 micrometers, higher signal-to-noise ratios, improved purge control, and enhanced stability for both vapor-phase and liquid-phase measurements. Compared to our previous instrument (Thermo Fisher Scientific® Nicolet™ 6700), the broader wavelength coverage enables characterization of longer-wavelength absorption features associated with aromatics, fuel additives, and other functional groups. The system is equipped with a heated optical cell capable of vapor-phase measurements up to 300 degrees Celsius and an Attenuated Total Reflectance (ATR) crystal cell for accurate analysis of liquid-phase samples.

Looking forward, these improvements will allow us to build a unified training set containing both vapor-phase and liquid-phase spectra for each fuel, evaluate how spectral phase influences property prediction performance, and ultimately develop a combined liquid–vapor modeling framework that delivers optimal accuracy across all fuel properties.

Milestone

- Presented reporting of experimental results and analysis at the Spring ASCENT meeting (April 2025).

Major Accomplishments

- Extended the FTIR-based compositional inference framework to predict thermochemical properties such as specific heat, enthalpy, and entropy.
- Evaluated and improved molecular-weight prediction performance using a new set of WJFS samples.
- Compared raw spectra, PCA-reduced spectra, and spectral moments to assess how spectral representations influence model accuracy and robustness.
- Set up and began operating the new Nicolet iS50 FTIR spectrometer, enabling expanded spectral measurements and improved data quality.

Publications

Peer-reviewed journal publication

Boddapati, V., Ferris, A. M., & Hanson, R. K. (2024). Predicting the physical and chemical properties of sustainable aviation fuels using elastic-net-regularized linear models based on extended-wavelength FTIR spectra, *Fuel, 356*, 129557. https://doi.org/10.1016/j.fuel.2023.129557

Outreach Efforts

Our thermochemical property prediction work was presented at the Spring ASCENT SAF Meeting (April 23-24, 2025),

Awards

None.

Student Involvement

Graduate students are actively involved in the acquisition and analysis of all experimental data and model development. Andrew Klingberg (current graduate student) and Miguel Figueroa Labastida (current postdoctoral fellow) performed the IR spectral analysis/fuel prescreening. Jesse Streicher (current research scientist) has additionally contributed to the project through research management.

Plans for Next Period

- Continue to expand the training dataset by adding FTIR spectra and property data for additional hydrocarbons across a broad range of molecular classes.
- Acquire and analyze additional SAF samples with varied compositions to further validate and refine the property-prediction strategies.
- Compile paired vapor-phase and liquid-phase FTIR spectra for each fuel to create a unified training set.
- Develop an integrated liquid–vapor modeling framework that achieves optimal predictive accuracy for all targeted fuel properties.