Project 033 Alternative Fuels Test Database Library

University of Illinois at Urbana-Champaign

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- P.I.: Tonghun Lee, Professor
- FAA Award Number: 13-C-AJFE-UI-038
- Period of Performance: October 1, 2024, to September 30, 2025
- Tasks:
  1. Online database development
  2. Chemical kinetic mechanism development

Project Funding Level

Federal Aviation Administration (FAA) funding level: $150,000
Cost-sharing: Software license support from Reaction Design (ANSYS)

Investigation Team

Tonghun Lee (P.I.), All Tasks
Emily Grinage (Graduate Student), All Tasks

Project Overview

This study continues development of a data library (Alternative Jet Fuels Test Database [AJFTD]). The functions of this database are (1) to serve as a comprehensive repository of conventional and sustainable aviation fuel (SAF) test data for the commercial aviation sector and (2) to provide fuel analysis techniques applicable to the rapid assessment and prescreening of novel SAFs. Currently, the repository comprises over 24,000 fuel samples and their respective test data, available for download to approved users of the project website. Figure 1 shows the main database web portal, currently housed at the University of Illinois at Urbana-Champaign (https://altjetfuels.illinois.edu). Database data include results from national laboratories, research efforts, airports, and other sources. In 2020, all compiled database data were converted to a new nonstructured query language (NoSQL) format by using a JavaScript® object notation (JSON) schema. This nonrelational structure allows the data to be analyzed using a variety of computational codes.

The catalog of data currently available in the database is primarily assembled from four separate sources. Fuels with POSF (Air Force Research Laboratory fuel database code) number designations were added from the internal database maintained by the Air Force Research Laboratory at Wright Patterson Air Force Base. The second dataset was obtained from Petroleum Quality Information System reports of the Naval Air Systems Command and corresponds to a compilation of fuel data primarily geared for government use. The third set was provided by Metron Aviation, consisting of fuel properties from samples collected at airports through a previous ASCENT project. The dataset resulting from this study has proven

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valuable by showing the landscape of fuels currently used in commercial aviation and will guide our future efforts focused on capturing this type of data in real time. The final dataset was obtained from the National Jet Fuel Combustion Program within ASCENT.

Though the database already contains a uniquely large collection of publicly available jet fuel data, data collection efforts are ongoing. Data collection is continuing to be pursued both domestically, focusing on airport and United States (U.S.) refinery data, and internationally, focusing on European sustainable aviation programs. The database documents SAF development and usage trends globally to increase understanding of global fuel infrastructure and variability. Multiple tools for fuel analysis have been implemented on the project website over the years to aid researchers in understanding SAFs. Machine learning techniques for fuel property analysis have been developed. More recently, a graphical interface for assessing fuel two-dimensional gas chromatography (GCxGC) composition information was added to the website. Analysis efforts now encompass the determination of suitable surrogate fuels to model novel SAFs and the rapid development of chemical kinetic models to predict behavior of SAFs in combustion regimes.

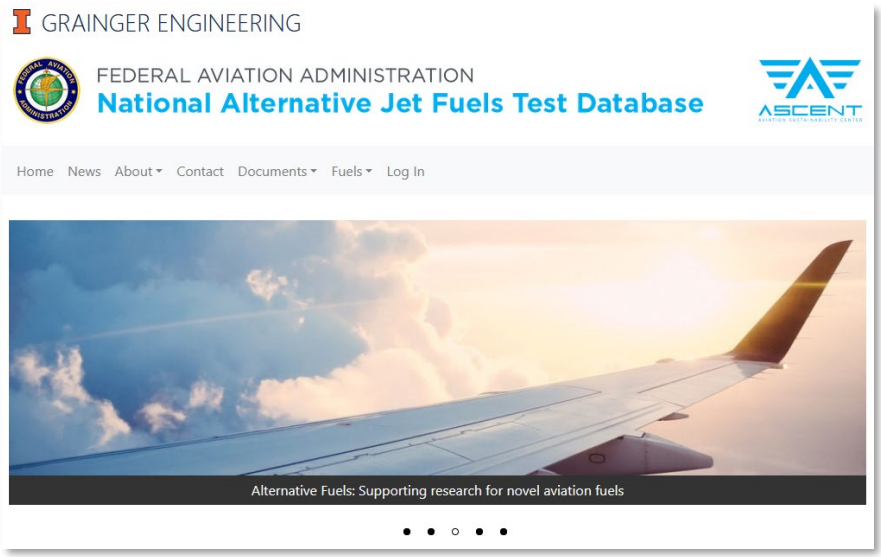

Figure 1. Alternative Jet Fuels Test Database (AJFTD) main webpage (altjetfuels.illinois.edu).

The current goals for the website include:

- Developing a common data schema and storage protocols with the World Fuel Survey.
- Strengthening connections with domestic airports for ongoing real-time data sharing.
- Initiating data sharing with international programs such as ALIGHT and NewJET.
- Developing and refining a methodology for chemical kinetics development based on website data.

Task 1 focuses on data collection and website development efforts, while Task 2 elaborates on the development of an analysis tool for inclusion on the database website.

Task 1 – Online Database Development

University of Illinois at Urbana-Champaign

Objectives

The main objective of this task was to expand and improve the database and its website. Currently, AJFTD is the second generation of the project website, with new capabilities and improvements consistently being added. Bugs are fixed as they are discovered, and improvements to the user interface and ease of data access are constant considerations. Data

acquisition efforts continue to obtain new data for inclusion on the database. The main Task 1 objectives are summarized as follows:

- Upgrade user interface to aid in the access of fuel data.
- Debug interface where needed.
- Establish fuel data sharing with target domestic airports.
- Establish fuel data sharing with U.S. refineries and other fuel sources.
- Forge connections with European programs such as ALIGHT and NewJET.

Research Approach

Website Upkeep

An integral part of website upkeep is building administrative tools to refine the user experience over time. To that end, new administrative capabilities were introduced this year to monitor user activity. These new features track site traffic, search behavior, and filter usage, providing invaluable metrics for maintaining reliability and relevancy site wide.

- **Fuel Search and Download Logs.** Administrators can now monitor which fuels are searched and downloaded. This information gives detailed context of what information is relevant to users and can help steer further database improvements.
- **Unique User Activity.** Administrators can track the number of unique users logged in to the database on a daily or weekly basis. This information is a useful metric to confirm the relevancy of the database.

Figure 2 shows a summary of the weekly activity for the National Alternative Jet Fuels Test Database.

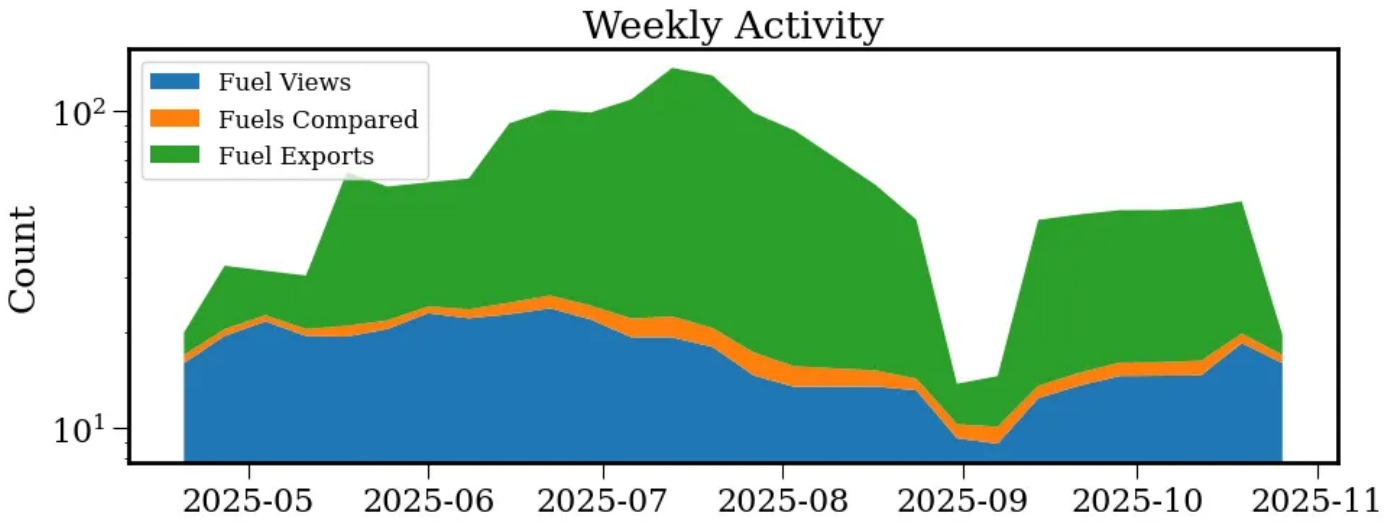

Figure 2. Database Activity Summary.

New administrator functions will continue to be developed, allowing administrators more power to customize website features for the benefit of users.

Website Upgrades

An effective user interface is essential to streamline access to relevant fuel data and support impactful research. Improvements are consistently considered and implemented. Last year, a large effort went into improving the fuels search page. The page now loads quickly, displaying only 10 fuels per page by default. Streamlined search filters appear on the left, featuring dropdown, multi-select, and intuitive buttons to control search updates (see Figure 3). Users can view individual or multiple fuels at a time with the 'Compare Selected' option. While the redesign significantly improved usability, inconsistent formatting in legacy data left some fuels improperly tagged for relevant searches. This year, tags were standardized across all fuel entries to ensure alignment with the search filters.

In the database's second generation, fuel entries were migrated from standard Certificates of Analysis (CoA) tables to structured JSON format to ensure compatibility with JETSCREEN. Storing each entry as structured JSON rather than tabular records improves interoperability and enables more efficient processing, including the search filtering schema. Most search filters mapped cleanly to existing JSON fields, however not all JSONs had an explicit entry for fuel class. The fuel classes in this filter include Alternative, Blend, Conventional, Engineered, and Sustainable Aviation Fuel. For some data sources like airport data, the fuel class "Conventional" is implied, but was not explicitly stated or tagged as such in the respective JSON files. Therefore, if a user were to search under this filter, the search results would not include all relevant fuels. To resolve this, the dataset was audited and backfilled, so all fuel entries are explicitly tagged, and a required "fuel_class" field with a controlled vocabulary is now enforced for all imports.

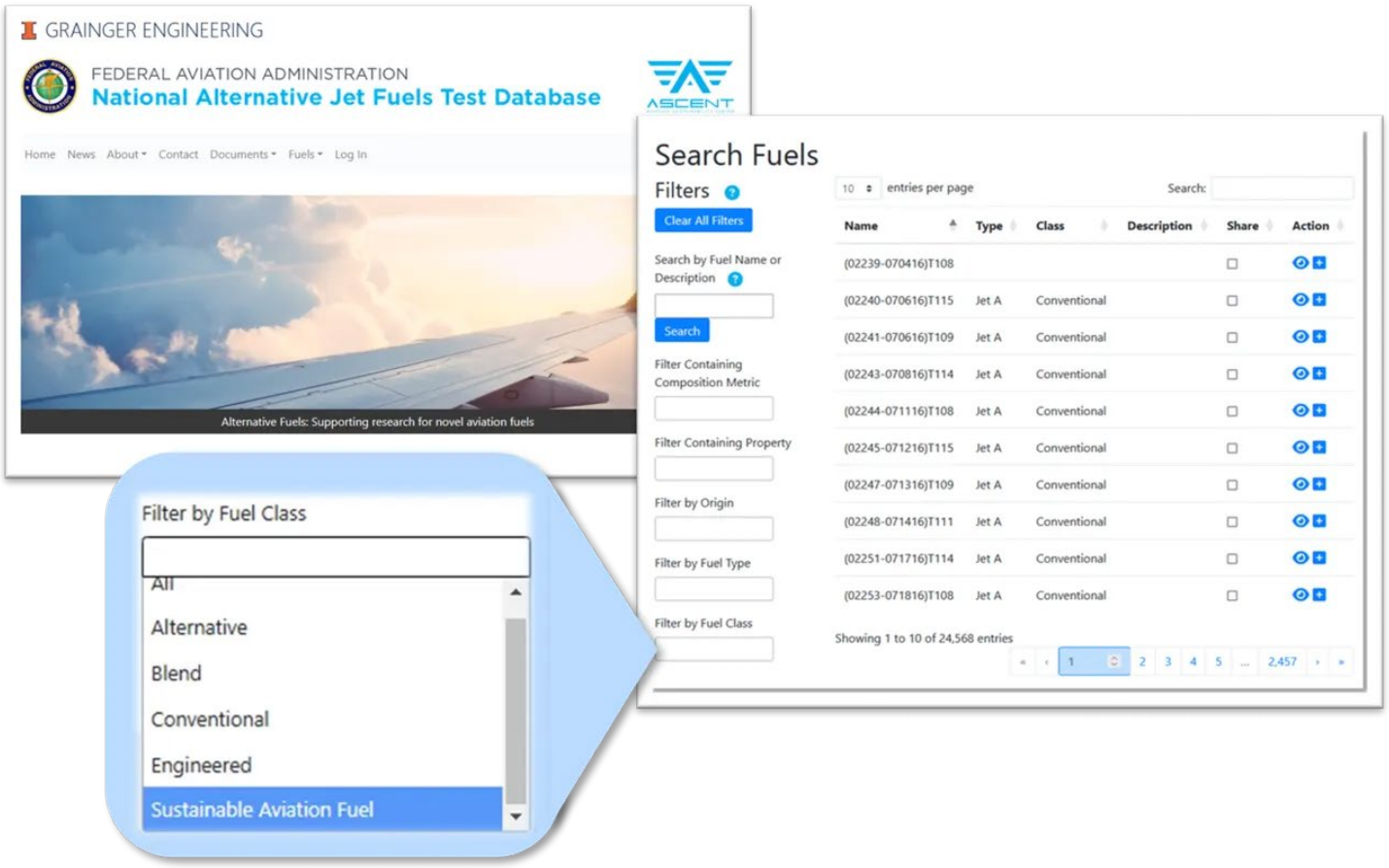

Figure 3. Fuel Class Filter on Search Page.

Airport Data Collection

AJFTD actively sources new data to capture trends in jet-fuel usage over time and region. In the past, 11 different domestic airports have provided fuel data to the database through a connection with Metron Aviation. These airports are indicated by black squares and their airport code in Figure 4. In the years since, our team has sought to establish robust connections with a few key airports in the U.S. to set up a foundation for real-time data sharing. The targeted airports are the Chicago O'Hare International Airport (ORD), Seattle-Tacoma International Airport (SEA), San Francisco International Airport (SFO), Daniel K. Inouye International Airport (HNL), and airports in the New York city region, which are governed by a common port authority. In the prior year, datasets from SFO (2021–2023) and SEA (2023) were received. These datasets are going through the standard pipeline of format conversion and vetting for integration onto the database. Communication has been sent to HNL and the New York Port Authority, and some progress has been made in obtaining data. These efforts are ongoing and will continue in the next year.

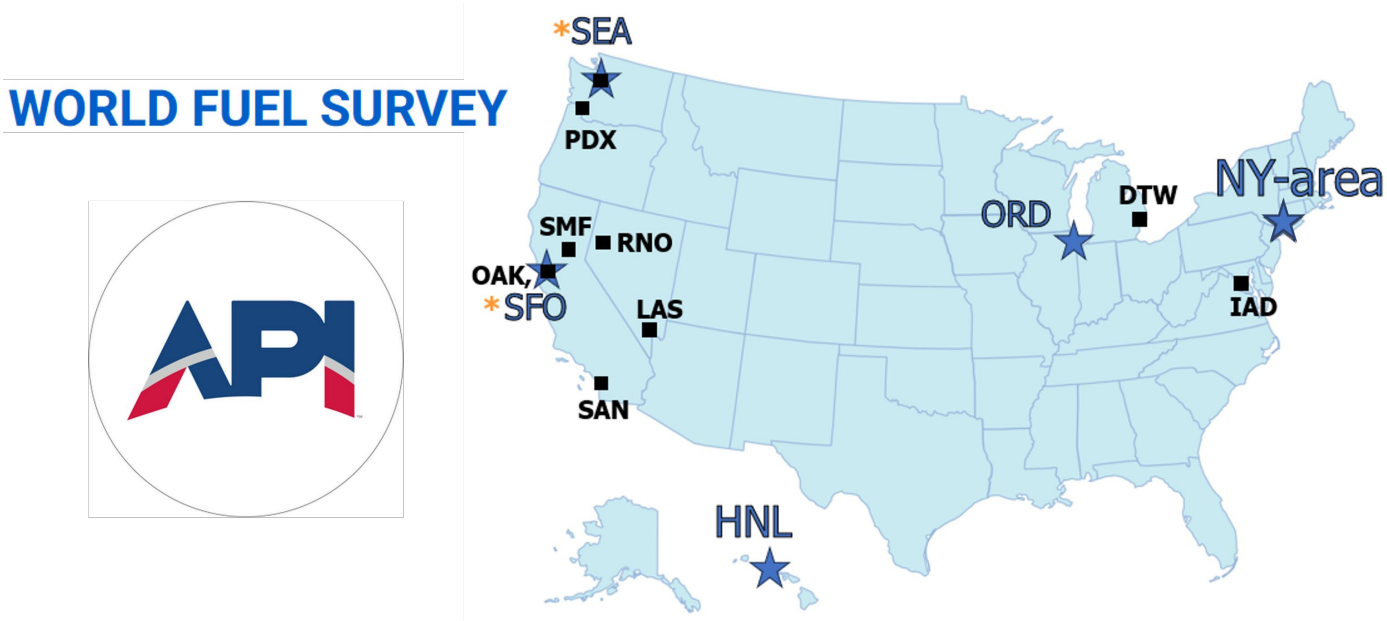

Figure 4. Data Collection Targets for Project Year.

World Fuel Survey
This project year involved connection and collaboration with ASCENT Project 090: World Fuel Survey. Meetings with the Volpe National Transportation Systems Center and University of Dayton Research Institute were held to establish a common data storage method and to begin aligning data formats across projects. The World Fuel Survey data informs international jet fuel production and property trends. While it will be published as a standalone set, it will also be integrated into the database once it is approved for public release. Its addition will expand the scope and diversity of fuels represented. One day, these projects may be integrated into one common database under the FAA, and coordinating data structure among the projects will help streamline that process and reduce the need for extensive reformatting in the future.

API 2022 Jet Fuel Survey
Early this year, connections were established with the Fuel Technologies Team Lead conducting a survey of 2022 CoA/Refinery Certificates of Quality from various American Petroleum Institute (API) refineries nationwide. Phase I of the survey was completed in April 2025 and resulted in the collection of over 25,000 CoAs. The volume of these data has significant impact, nearly doubling the database's existing fuel entries and broadening the range of fuels represented. This survey is ongoing, as API continues to collect data from 2023 onward. The magnitude of this data volume has also highlighted potential improvements to the importer framework of AJFTD to make future data integration as seamless and efficient as possible.

Research Program Data Collection
In addition to U.S. sources, connection with European programs provides valuable breadth to the database. The AJFTD's past connection with JETSCREEN in Europe established a foundation for data sharing with international programs and showed the value of cross-regional collaboration. European programs (ALIGHT and NewJET are our current targets for data collection overseas, as they focus on SAF deployment and aviation emissions). Last year marked the first time a representative from the AJFTD attended the ECATS conference in Europe to share information about the database, present its capabilities to a broader audience, and initiate connections with representatives of ALIGHT and NewJET. This outreach increased international visibility of the database and opened new opportunities for collaboration. Strengthening these connections and converting initial discussions into active data-sharing efforts is an ongoing priority of the project.

Milestones

3 months

- Followed up with representatives at HNL.
- Connected with API Jet Fuel Survey Taskforce.
- Established data storage options with World Fuel Survey.

6 months

- Added new administrator functionality to the AJFTD.
- Standardized fuel tagging across all data entries.
- Presented updates at the Spring SAF ASCENT meeting.
- Received final dataset from API 2022 Jet Fuel Survey.

9 months

- Identified new target airports for data collection.
- Began CoA to JSON conversion for new datasets.

12 months

- Presented updates at the Fall 2025 ASCENT meeting.

Major Accomplishments

Connections with API, the World Fuel Survey, HNL, and the New York Port Authority have been secured and are expected to lead to increased data collection in the coming years. In addition, new administrative tools and data formatting improvements will lead to improved usability of the database. Standardized data formatting and integration lays the groundwork for the implementation of more complex analysis techniques in the future, which will help shape the future of SAF in commercial aviation.

Publications

None.

Outreach Efforts

In both the Spring and Fall of 2025, project updates were shared at the ASCENT semiannual conferences. These presentations led to productive discussions regarding fuel data acquisition, database usage, and avenues for further outreach.

The database has been made accessible at https://altjetfuels.illinois.edu.

Awards

None.

Student Involvement

This project was primarily conducted by a graduate student, Emily Grinage.

Plans for Next Period

In the next period, the focus on data collection from target airports will be emphasized. Obtaining further data samples from HNL will be prioritized. In addition, the team will continue pursuing connection with the New York Port Authority to share our data collection vision. Meetings with ALIGHT and NewJET leaders are anticipated as well.

The improvement of the database website will continue with efforts such as:

- **Search interface refinement.** The new fuels search page will continue to be tested to assure the feature is free of bugs. Minor improvements will continue to be made.
- **Improved analysis tools.** A tool to rapidly generate kinetic mechanisms for further jet fuel performance analysis is underway. Implementation of this analysis feature will begin in the next term.

Task 2 – Chemical Kinetic Mechanism Development

University of Illinois at Urbana-Champaign

Objectives

The objective of this task is to evaluate approaches for rapidly generating chemical kinetic mechanisms for aviation fuels, for eventual integration into AJFTD. Such mechanisms are essential for combustion simulations (e.g., computational fluid dynamics) which significantly decrease time and cost to certify new fuels. As SAFs become more prevalent, timely mechanism development becomes critical. However, building and reducing detailed mechanisms can demand significant computational time and resources, especially for emerging fuels with uncertain properties. Accelerated, reliable methods for constraining and generating mechanisms are essential for broader SAF adoption. This effort examines these methods and opportunities for improvements. The major goals of this task are:

- Outline and implement a robust methodology for the rapid development of mechanisms for any novel SAF with limited experimental data.
- Demonstrate selected approach in mechanism generation for CycloSAF.
- Quantify uncertainties and effectiveness of the constraining approach.

Research Approach

Methodology

New SAFs are initially produced in very small fuel volumes. Fuel producers are reluctant to scale fuel production to commercial quantities until the SAF has been approved and certified for use on an existing aircraft. Prescreening with combustion models is therefore critical for estimating FAA compliance and informing investment decisions. Given the limited volumes of fuel available, such models must be accurate while relying on as little experimental data as possible. Commonly used experimental data include GCxGC and ignition delay time measurements. GC×GC can extract detailed compositional information from small samples, which provides the basis for the mechanism-development approach presented here.

The methodology for mechanism determination outlined for 2025 is summarized in Figure 5. This approach is an expanded version of a general methodology outlined in the year prior. GCxGC data gives details about a fuel's composition, which informs the creation of an appropriate surrogate fuel to model a SAF of interest. Surrogate determination for SAFs with novel compositions can be particularly difficult, especially if there is limited literature on the specific hydrocarbons that make up the fuel. To make use of the abundance of kinetics research in a way that is applicable to hydrocarbon behavior that has not been carefully studied, a generalized approach using a fuel's functional groups was developed.

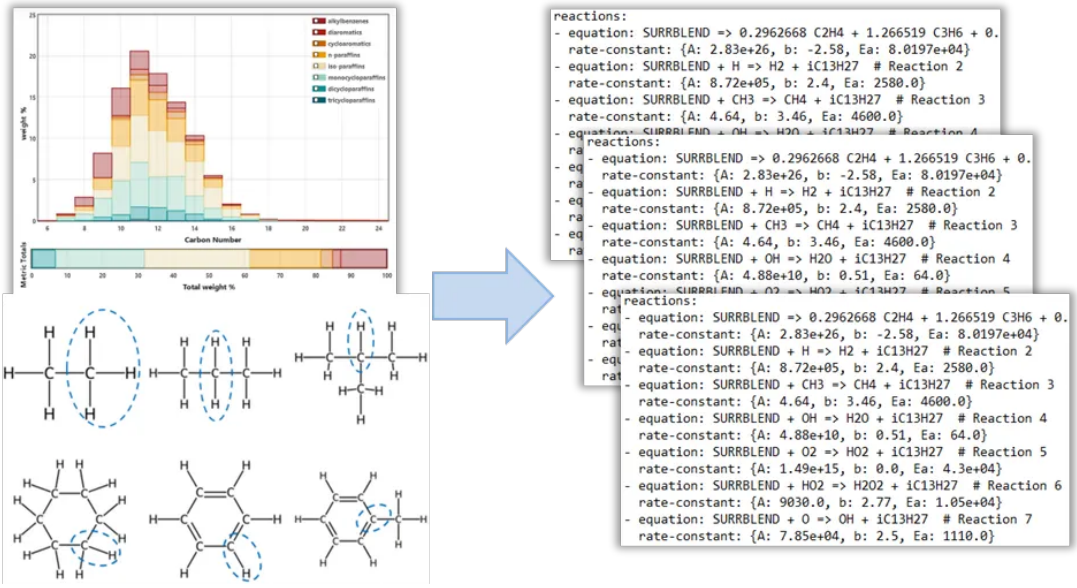

Figure 5. General kinetics approach: transforming Fuel GCxGC data into a mechanism using Chemical Functional Groups.

Figure 6 provides a more detailed overview of the generalized approach for mechanism determination for any SAF. If the fuel's composition is known, a surrogate can be formulated to closely match the properties of the actual fuel. Once a surrogate is created, established kinetic mechanisms are used to simulate the breakdown of the surrogate in various combustion environments, such as shock tubes or plug flow reactors. The results from these simulations inform the stoichiometric coefficients for a set of reactions that govern the initial breakdown of the chosen SAF and its primary decomposition pathways. This set of reactions forms the Hybrid Chemistry (HyChem) mechanism structure. Once the stoichiometric coefficients and rates of these breakdown reactions are determined, the new model is constrained towards experimental data to determine which experiments are most critical in rapidly developing mechanisms for new SAFs.

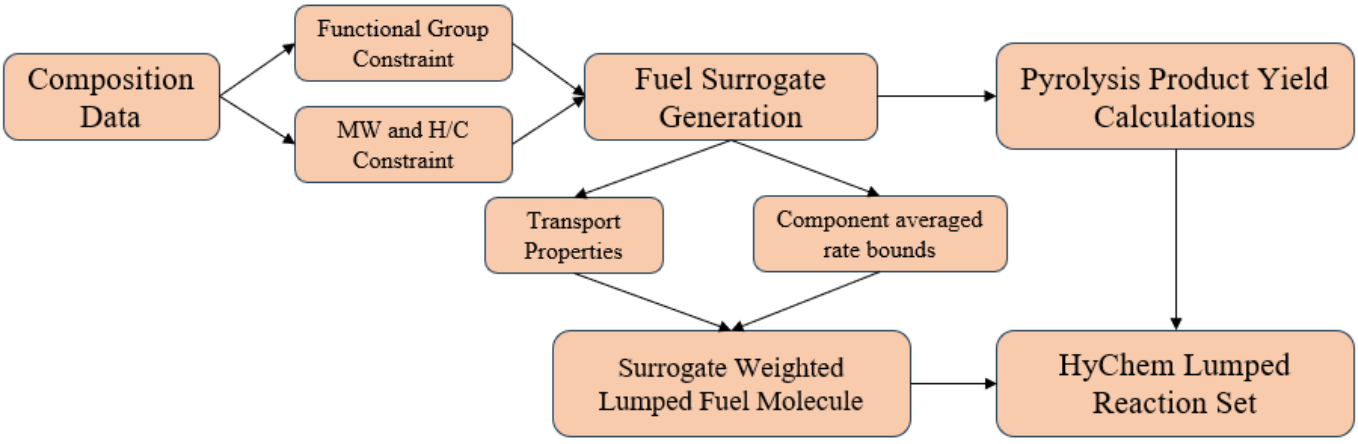

Figure 6. General methodology to generate kinetic mechanism for any fuel

Preliminary Implementation

The feasibility of this method was tested last year by creating a mechanism for an alcohol-to-jet (ATJ) fuel manufactured by

Gevo® (POSF 11498). ATJ was chosen due to the availability of experimental data for this fuel in the literature. The current approach has been modified to broaden its applications to fuels with limited data available, as this is the case for most new SAFs being prescreened for certification. This improved approach will be demonstrated by creating a mechanism for CycloSAF, a fuel manufactured by CleanJoule.™ CycloSAF is unique in that it is made up almost entirely of 10-carbon cyclo-alkanes. The certification of such a fuel would have significant impact on SAF requirements. ASTM 7566 (ASTM, 2023) currently requires SAF's to include 8% aromatics to ensure proper volume swell characteristics needed for O-ring compatibility in the jet engine. Cyclo-alkanes exhibit volume swell properties similar to aromatics while producing substantially less soot. Like many SAFs early in the certification pipeline, there is very limited experimental data and literature available on CycloSAF's behavior. This presents a unique challenge in the previously developed surrogate fuel modeling approach.

To perform simulations on a surrogate fuel, the surrogate must be comprised of species that are already modeled in an existing kinetic mechanism. Many existing detailed mechanisms have been designed for jet fuels made primarily of normal-alkanes and iso-alkanes. Some cyclo-alkanes are represented, but there are no existing mechanisms with large cyclic species like those in CycloSAF. Instead of modeling the surrogate fuel with C10 cyclo-alkanes, it can be modeled to match the functional groups that would be found in the fuel. Functional groups of hydrocarbon species can be determined from nuclear magnetic resonance (NMR) or estimated from GCxGC data. This surrogate modeling approach has been used in several research efforts, namely the creation of FGMech, a mechanism generation method used and validated for 14 surrogate fuel mixtures and 12 real fuels (Zhang & Sarathy, 2020). Functional group matching has been shown to reasonably capture ignition and combustion characteristics. As a result, functional-group-based surrogates can be used as an additional constraint when generating surrogates for novel compositions.

CycloSAF is primarily made up of three cyclo-alkane species that are not in any existing chemical kinetic mechanisms. Both Dimethylcyclo-octane (DMCO) species have an 8-carbon ring and two methyl groups. Para-menthane is a 6-carbon ring with 3 methyl groups and an additional carbon branch. Details on these species structures and functional groups present can be seen in Figure 7. The weight percents of respective functional groups were used as a constraint in generating a surrogate fuel, in addition to matching molecular weight and hydrogen-to-carbon ratio. Functional groups contain key information about how a fuel molecule will break down. Constraining the surrogate to the fuel's functional groups preserves site-specific bond breaking behavior, and conserves hydrogen/carbon (H/C) ratio. Matching molecular weight ensures that transport properties like density, viscosity, and diffusion are modeled properly. While matching the functional groups of a fuel in a surrogate model is a good approximation for the local bond behavior, it does not consider global molecular effects like ring strain. Because of this uncertainty, a distribution of 1,000 fuel surrogates was created to further understand how these effects would propagate through the mechanism generation pipeline. This uncertainty analysis is still in process, but the remaining steps in this methodology use the surrogate fuel composition that most closely matches experimental data for ignition delay time.

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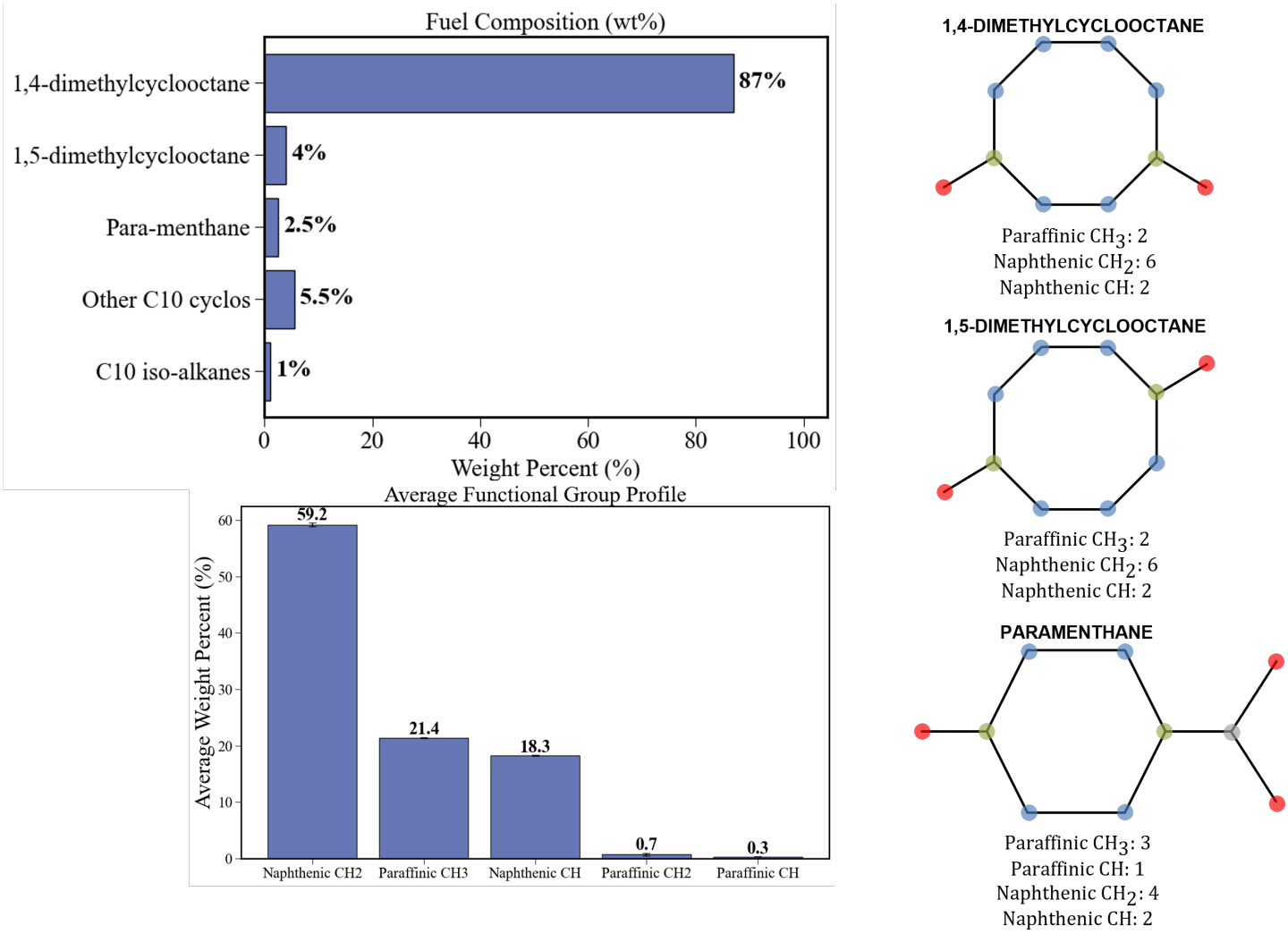


Figure 7. CycloSAF composition and species functional groups.

Once a surrogate fuel model has been constructed, the fuel can be used in various simulated combustion events to further develop our kinetic mechanism. A HyChem structure was adopted for the mechanism determination approach. In this structure, the fuel is treated as one "lumped" fuel molecule with properties representative of the fuel of interest. A set of approximately 20 reactions describe the breakdown of this "lumped" fuel molecule into smaller hydrocarbon products, or pyrolysis products. From here, a large, descriptive model applicable to any jet fuel handles reactions of these smaller hydrocarbons. For HyChem, this large model is the USC-II[1] mechanism.

The creators of HyChem postulated that most jet fuels have the same key pyrolysis products. Complex jet fuels will break down into many different hydrocarbons, but of these, only about eight smaller hydrocarbon species will be strongly present and will govern the behavior of the post-pyrolysis species mixture. Then, for any new SAF of interest, a researcher need only determine which of these key products are produced from the pyrolysis of the SAF, and what the ratios of the products are to one another. The creators of HyChem determined these pyrolysis products by conducting extensive plug flow reactor and shock tube experiments and directly measuring or calculating product concentrations (Wang et. al.,

[1] The USC II mechanism was developed at the University of Southern California by Professor Hai Wang. This mechanism aims at representing a wide variety of combustion scenarios.

2018). For the purposes of this project, the goal is to avoid using the high fuel volumes and long experimentation times necessary to conduct these tests. Instead, the plug flow reactor and shock tube experiments were simulated as closely as possible using Cantera[2] simulations. Cantera simulation inputs were the previously determined surrogate blend for CycloSAF.

The Cantera simulation results for the CycloSAF surrogates were used to determine which of the key pyrolysis products were represented and their ratios to one another. This information fed into the mechanism structure in the form of the stoichiometric coefficients of fuel-specific reactions governing the high- and low-temperature breakdown of the lumped fuel molecule. Two sub-mechanism variants were evaluated: (i) a 16-reaction structure, consistent with the prior ATJ mechanism, and (ii) a 20-reaction set that adds an additional H-abstraction reaction ($Fuel \rightarrow R + H$)and low-temperature pathways ($ROO \leftrightarrow Q + HO_2, QOOH \rightarrow QO + OH,\ QO + OH \rightarrow Pyrolysis\ Products$). The additional reactions in sub-mechanism (ii) were included because comparisons with detailed kinetic mechanisms show that H-abstraction and alkylperoxy/ hydroperoxyalkyl radical (ROO/QOOH) conversion are dominant low-temperature channels for cycloalkane fuels.

At this point, the HyChem CycloSAF mechanism had been modified only in terms of stoichiometric coefficients in the reactions, and not in terms of the reactions' rates. In the previous approach (2024), rates of the lumped fuel breakdown reactions were determined using a Hybrid Response Surface Network followed by a Stochastic Gradient Descent Ensemble (HRSN-SGDE) approach. This approach has been described in more detail in past reports and publications by UIUC (Oh et al., 2023; Wiersema et al., 2024a; Wiersema et al., 2024b). This machine learning approach can rapidly estimate ignition delay measurements instead of calculating them from a set of input conditions. While this model can quickly output sets of reaction rate coefficients that will satisfy ignition delay data, training the model for every novel SAF is not ideal. For this reason, another approach was taken for reaction rate approximation. The HRSN-SGDE approach can still be used for rate refinement if necessary.

To quickly approximate the reaction rates for the HyChem structure reactions, an effective rate constant was calculated from corresponding reaction rates of the surrogate component fuels. For example, take the reaction:

$$\mathrm{CycloSAF} \rightarrow e_d\left(C_2H_4 + \lambda_3 C_3H_6 + \lambda_{\{4,1\}} C_4H_8 + \lambda_{\{4,i\}} iC_4H_8\right) + b_d[\chi C_6H_6 + (1\text{-}\chi)C_7H_8] + \alpha H + (2\text{-}\alpha)CH_3$$

This reaction describes the breakdown of the CycloSAF lumped fuel molecule into pyrolysis products. The variables e_d, λ_i, b_d, χ, α are determined from the prior shock tube and plug flow reactor simulations. To approximate the rate at which the above reaction takes place, a weighted average of corresponding surrogate component rates was conducted.

This effective rate constant for this reaction would then be (Equation 1):

$$\sum_i X_i k(T)_i \qquad \text{(Eq. 1)}$$

where i = all species in the surrogate fuel composition, X_i is the mole fraction of each surrogate component, and $k(T)_i$ is its respective rate function for the reaction of reach respective surrogate component breaking down to pyrolysis products.

The colored lines in Figure 8 show the respective rate functions for the breakdown of each surrogate component into pyrolysis products. The dotted line is the calculated effective rate for the CycloSAF lumped fuel molecule for different temperatures ranging from 500 to 2500 K. Arrhenius parameters A, Ea, and n are fitted to this effective rate curve. This procedure is done for every reaction in the lumped HyChem sub-mechanism to generate a consistent set of rates for the surrogate fuel.

[2] Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Cantera is a sponsored project of NumFOCUS®, a 501(c) nonprofit charity in the U.S. NumFOCUS is a registered trademark of NumFOCUS, Inc., Austin, Texas.

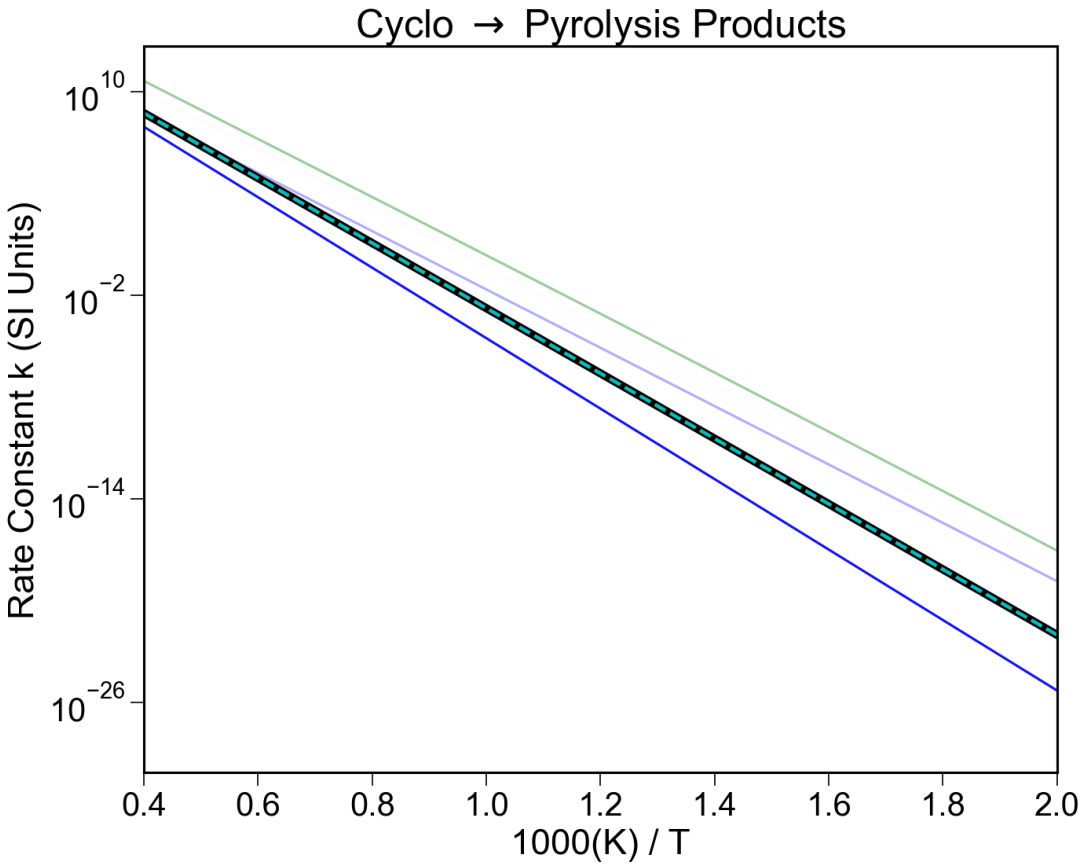
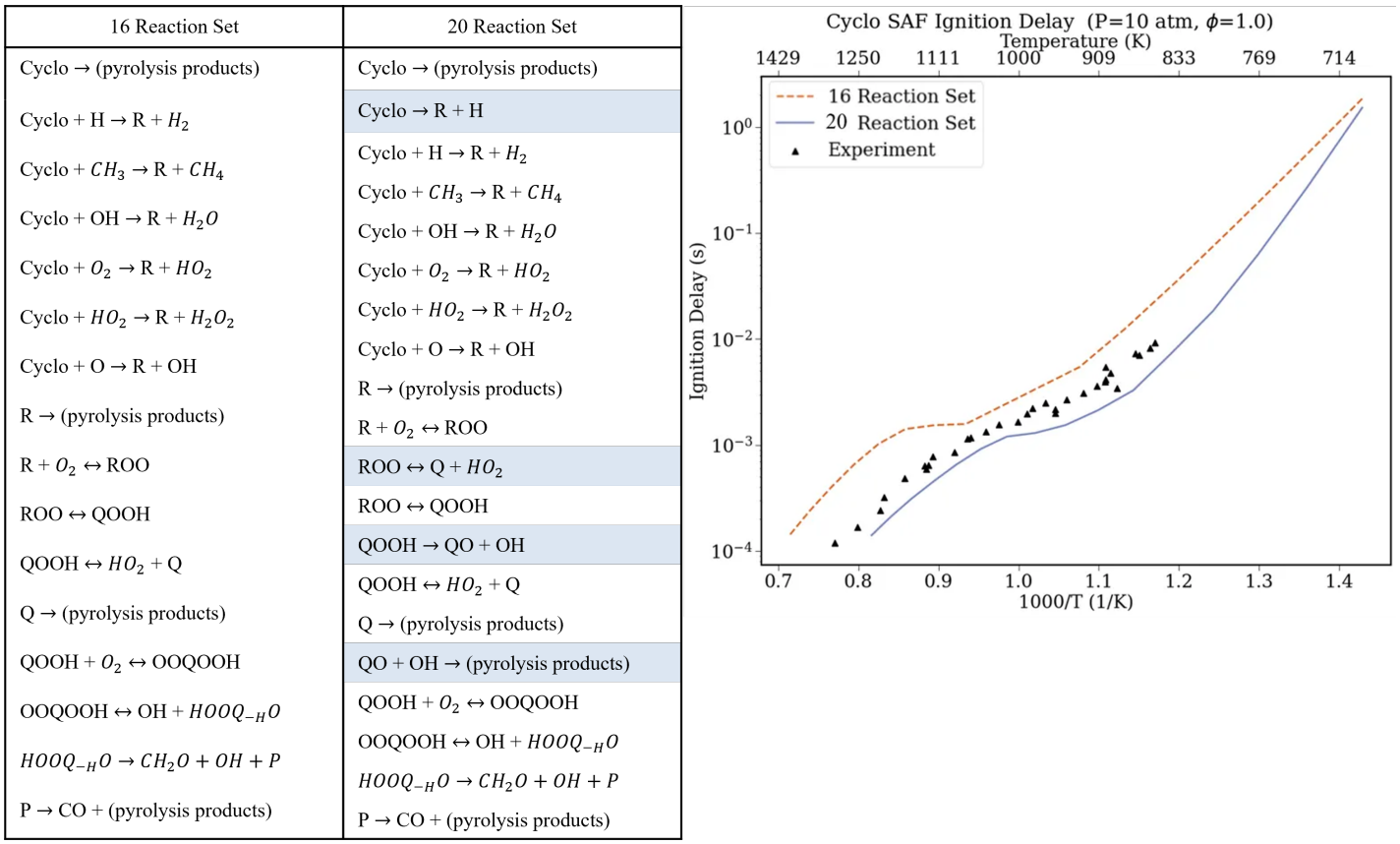


Figure 8. Surrogate Component and Lumped Fuel Molecule Rate Comparison.

Once the reaction rate parameters of our two sub-mechanism variations are complete, the resulting kinetic mechanisms were used to simulate ignition delay time across a wide temperature range, 700 to 1400 K. These results are displayed in Figure 9. The mechanism with 20 lumped pyrolysis reactions seems to underpredict ignition delay time, and the smaller sub-mechanism overpredicts. The Rapid Compression Machine needed to collect low temperature ignition delay data for CycloSAF has been at capacity, but once these data have been collected, further investigation will be performed to refine reaction rate parameters and investigate uncertainties. This methodology shows promise in its ability to approximate combustion parameters like ignition delay time for any fuel with known composition and basic combustion data. Because it does not rely on machine learning or large optimization routines, it can be scaled into a fast-running tool within the database framework.



16 Reaction Set	20 Reaction Set
Cyclo → (pyrolysis products)	Cyclo → (pyrolysis products)
Cyclo + H → R + H_2	Cyclo → R + H
Cyclo + CH_3 → R + CH_4	Cyclo + H → R + H_2
Cyclo + OH → R + H_2O	Cyclo + CH_3 → R + CH_4
Cyclo + O_2 → R + HO_2	Cyclo + OH → R + H_2O
Cyclo + HO_2 → R + H_2O_2	Cyclo + O_2 → R + HO_2
Cyclo + O → R + OH	Cyclo + HO_2 → R + H_2O_2
R → (pyrolysis products)	Cyclo + O → R + OH
R + O_2 ↔ ROO	R → (pyrolysis products)
ROO ↔ QOOH	R + O_2 ↔ ROO
QOOH ↔ HO_2 + Q	ROO ↔ Q + HO_2
Q → (pyrolysis products)	ROO ↔ QOOH
QOOH + O_2 ↔ OOQOOH	QOOH → QO + OH
OOQOOH ↔ OH + $HOOQ_{-H}O$	QOOH ↔ HO_2 + Q
$HOOQ_{-H}O$ → CH_2O + OH + P	Q → (pyrolysis products)
P → CO + (pyrolysis products)	QO + OH → (pyrolysis products)
	QOOH + O_2 ↔ OOQOOH
	OOQOOH ↔ OH + $HOOQ_{-H}O$
	$HOOQ_{-H}O$ → CH_2O + OH + P
	P → CO + (pyrolysis products)

Figure 9. CycloSAF HyChem Mechanism Comparison – Ignition Delay Time.

Milestone

3 months
- Identified areas of improvement to existing methodology.

6 months
- Outlined generalizable surrogate fuel modeling approach with functional groups.
- Identified an appropriate existing model for running surrogate simulations for CycloSAF.

9 months
- Determined surrogate fuel model for CycloSAF.
- Conducted surrogate simulations to emulate original HyChem methodology.
- Set up additional simulation framework from updated HyChem methodology to model low temperature pathways.
- Estimated reaction stoichiometric coefficients for fuel breakdown reactions.

12 months
- Simulation and comparison of initial CycloSAF mechanisms.
- Begin packaging scripts into one adaptable tool.

Major Accomplishments

A repeatable and significant methodology for rapid development of chemical kinetic models based on limited experimental data has been outlined and tested on a SAF with novel composition. A new surrogate modelling approach has been created based on the chemical functional groups of a fuel. Two variations of kinetic mechanisms for CycloSAF have been created and are being further refined as more data becomes available. Methods have been outlined to quantify the uncertainties in mechanism determination in future work.

Publications
None.

Outreach Efforts
In Spring and Fall of 2025, project updates were shared at the ASCENT semiannual meetings. These presentations led to productive discussions regarding fuel data acquisition, database usage, and avenues for further outreach.

Awards
None.

Student Involvement
This project was primarily conducted by one graduate student (Emily Grinage).

Plans for Next Period
In the next period, work will continue with the mechanism determination approach. Attention will be paid to the following areas:

- **CycloSAF model analysis.** Overall, the mechanism determination approach has been demonstrated with CycloSAF with reasonable agreement with experimental data, however there is room to further refine the model to low temperature data once it becomes available. Additional methods for improving rate calculations for the lumped pyrolysis reactions will be explored.
- **Uncertainty Quantification.** The functional group surrogate fuel modelling approach does not account for global molecule behavior, such as ring strain, etc. Uncertainties in model performance due to this approximation need to be further quantified and reduced.
- **AJFTD Implementation.** However, aspects of the approach have yet to be completely designed or implemented. Determining the stoichiometric coefficients of pyrolysis products is the bottleneck in this mechanism generation approach. Multiple simulations must be performed with the fuel surrogate using an existing detailed mechanism. The framework to host an equivalent tool on the website must be further investigated.

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