Project 24A:
Emissions Data Analysis for CLEEN, ACCESS, and Other Recent Tests

Massachusetts Institute of Technology

Project Lead Investigator

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- P.I.(s): Steven Barrett, Associate Professor
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- Task(s):
    - Task 1: Gather additional nvPM emissions data from recent measurement campaigns
    - Task 2: Update nvPM model to account for altitude effects
    - Task 3: Extend nvPM model to incorporate results from non-paraffinic alternative fuels

Project Funding Level

Project Funding Level: $95,000 FAA funding and $95,000 matching funds. Sources of match are approximately $4,000 from MIT, plus 3rd party in-kind contributions of $91,000 from Byogy Renewables, Inc.

Investigation Team

- Steven Barrett (Associate Professor, Principal Investigator, MIT) – Responsible for project management on all tasks.
- Raymond Speth (Research Scientist, Co-Investigator, MIT) – Responsible for Tasks 2 & 3 and coordination with ASCENT Project 24B research team at Pennsylvania State University.
- Robert Malina (Research Scientist, Co-Investigator, MIT) – Responsible for coordination with ASCENT Projects 20 and 21 and air quality and climate impacts.
- Luis Alvarez (Graduate Student, MIT) – Responsible for Task 1.

Project Overview

The objective of this research is to gather and analyze aircraft engine non-volatile particulate matter (nvPM) emissions data collected from CLEEN, ACCESS and other recent emission measurement campaigns and to develop improved models for the relationship between fuel composition and nvPM emissions. Improvements to estimates of nvPM emissions from alternative fuels will be useful in understanding the air quality and climate impacts of alternative jet fuels. The goals for this project are to expand modeling capabilities in the following areas:

- Extend the previously-developed ASAF (Approximation of Soot from Alternative Fuels) model (Speth et al., 2015) to account for changes in ambient conditions, i.e. adjusting for altitude to improve predictions of emissions at cruise altitude.
- Determine fuel properties that can serve as predictors of soot formation for fuels where the distribution of aromatic compounds differs from that found in conventional jet fuel
- Extend the ASAF model to allow predictions of nvPM from non-paraffinic alternative jet fuels, such as those produced by hydroprocessed depolymerized cellulosic jet (e.g. KiOR) or catalytic hydrothermal (e.g. Readijet) processes

Task 1: Gather additional nvPM emissions data from recent measurement campaigns

Objective(s)

This task consists of acquiring nvPM mass and/or number emissions measurements from recent measurement campaigns such as those conducted under the FAA CLEEN program and as part of the NASA ACCESS-2 study.

Research Approach

CLEEN Results

Results from the CLEEN program were extracted from the reports submitted to the FAA by Pratt & Whitney. These data consisted of nvPM mass emissions data collected at a range of thrust settings for a PW615F engine operated at sea level static conditions using the following fuels and fuel blends:

1. 100% Conventional Jet-A1
2. 30% KiOR hydroprocessed depolymerized cellulosic jet (HDCJ) / 70% Conventional
3. 50% KiOR hydroprocessed depolymerized cellulosic jet (HDCJ) / 50% Sasol FT
4. 20% Amyris direct sugar to hydrocarbon (DSHC) / 80% Conventional
5. 50% ARA catalytic hydrothermolysis (CH) / 50% Conventional
6. 100% ARA catalytic hydrothermolysis (CH)

For each fuel, the ASTM D1655 specifications for each fuel were also reported. At each operating point, we computed the relative emissions produced by the alternative fuel blend (compared to the conventional fuel operating at the same operating point) and the relative fuel aromatics content (compared to the conventional fuel aromatics content) and added these data to our database of alternative fuels emissions data. The original database consisted of equivalent test data collected for FT and HEFA paraffinic alternative fuels tested on 7 different turbofan and turbojet engines (not including the PW615F). The nvPM emissions from the alternative fuels tested under the CLEEN program are compared to the emissions from the FT and HEFA fuels is summarized in Figure 1.

ACCESS-2 Results

Through discussions with the principal investigator responsible for the ACCESS-2 campaign conducted by NASA, we were able to obtain preliminary results for some of the cruise-altitude nvPM measurements taken as part of this campaign. However, the currently available dataset only includes emissions for conventional jet fuel, and not any alternative fuel blends, and as such does not provide information which can be incorporated into our database.

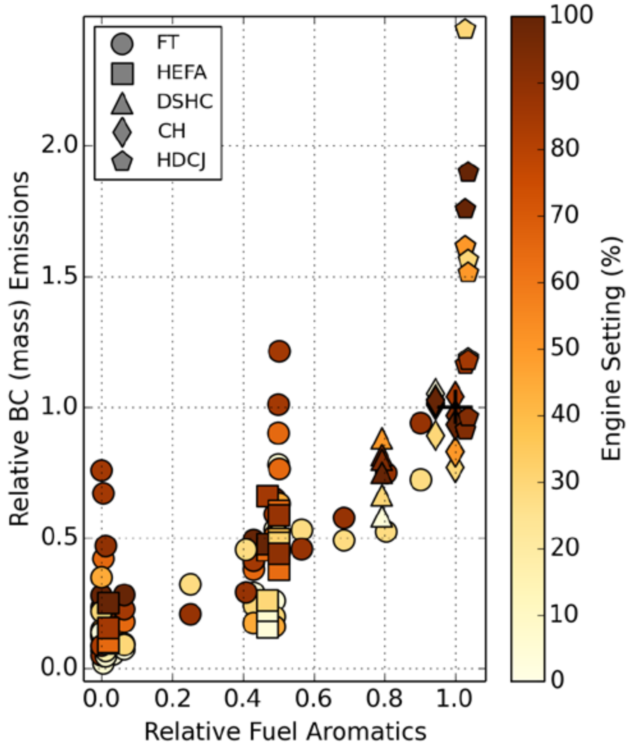

Figure 1: Relative BC emissions for different types of alternative fuels as a function of relative aromatics content and engine setting.

Milestone(s)

Milestone 1: Develop database of available emissions measurements and corresponding fuel properties for use in analyses

Major Accomplishments

The addition of the CLEEN measurements increases the breadth of the nvPM emission by adding three new fuel types, two of which (HDCJ and CH) have fuel compositions which are significantly different from previously-studied alternative fuel mixtures. This provides a foundation for improving on our alternative fuel nvPM predictive model to account for the more complex fuel compositions which are present in several alternative jet fuels of interest.

Outreach Efforts

These results were presented at the Aviation Emissions Characterization Workshop which was held May 19-20, 2015.

Student Involvement

Luis Alvarez was primarily responsible for gathering the emissions data from the CLEEN program and incorporating it into the existing emissions database.

Task 2: Update nvPM model to account for altitude effects

Objective(s)
The objective of this task is to extend the ASAF model to account for changes in ambient conditions, i.e. adjusting for altitude to improve predictions of emissions at cruise altitude, and to validate these modifications against the data collected in the ACCESS-2 study.

Research Approach
Since ground level nvPM measurements are much simpler than cruise-altitude measurements, the vast majority of emissions tests on alternative fuels have been conducted at sea-level static conditions. However, in order to evaluate the effects of cruise-altitude emissions on other atmospheric processes, e.g. contrail formation, these ground level test data must be mapped to cruise conditions. Previously, the correspondence between ground level and cruise altitude conditions was addressed in the FOX model (Stettler et al., 2013) for nvPM emissions from conventional fuels using a correlation developed by Döpelheuer and Lecht (1999). This correlation does not include any parameters which would account for different behaviors based on changes in fuel composition, and as such cannot account for any potential differences in the behavior of alternative fuels.

Because the ACCESS-2 alternative fuel measurements have not yet been made available, there is at present no experimental data on which to base an updated correlation relating ground-based alternative fuel emissions measurements to cruise altitude. Instead, we have pursued an approach based on using a chemical reactor network model with a detailed chemical kinetic mechanism (Ranzi et al., 2012) to predict formation of large polycyclic aromatic hydrocarbons (PAH) in the primary reaction zone, which are considered to be precursors to soot formation. This model was run for a range of engine conditions, covering variations in inlet temperature, inlet pressure, pressure ratio, equivalence ratio, primary reaction zone volume, and fuel composition. The parameter ranges included values which are expected to be relevant to both ground-level and cruise-altitude conditions.

Milestone(s)
Milestone 2: Provide FAA with a briefing on the model with altitude effects incorporated. This briefing was provided as part of the AEC Roadmap Teleconference on September 24, 2015.

Major Accomplishments
We found that for a range of fuel compositions, relative soot formation (compared to soot formation for a naphthalene, a high-sooting fuel) for ground and cruise conditions were similar when comparing cases where the burned gas temperature was held constant, rather than cases where the equivalence ratio was held constant. These results are summarized in Figure 2.

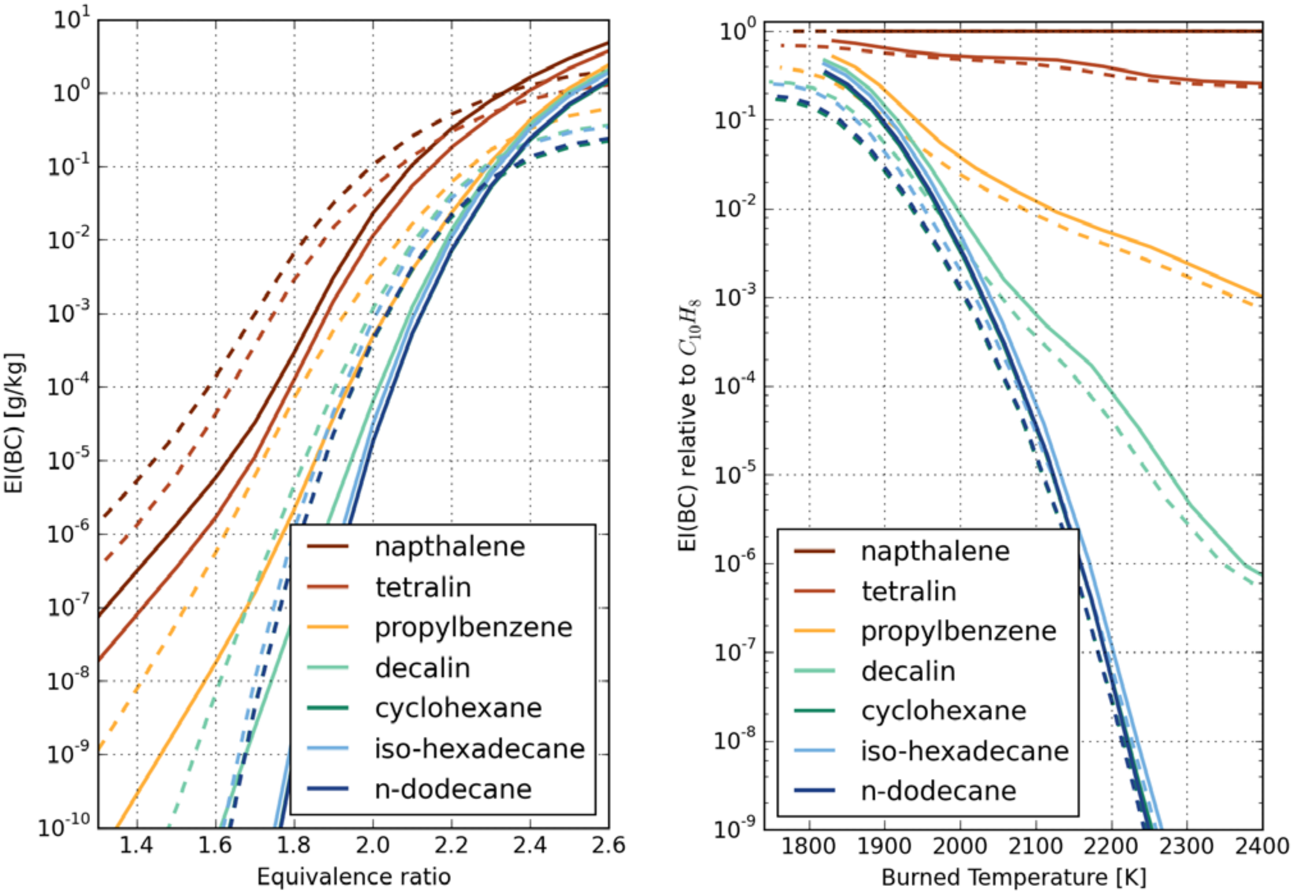

Figure 2: Comparison of black carbon emissions indices for selected fuels at ground level (solid lines) and cruise altitude (dashed lines). Left: Absolute emissions indices as a function of equivalence ratio. Right: normalized emissions indices as a function of burned gas temperature.

This correspondence of results suggests that ground-level, static emissions test sample the desired parameter space of engine operating conditions, and that correlating ground and cruise altitude emissions is feasible. However, some data on cruise altitude emissions needs to be used in order to develop and validate such a correlation.

Outreach Efforts

A presentation describing the analysis of altitude and fuel composition effects using the reactor network model was given in the AEC Roadmap Teleconference on September 24, 2015.

Task 3: Extend nvPM model to incorporate results from non-paraffinic alternative fuels

Objective(s)

The objective of this task is to extend the ASAF model to allow predictions of nvPM from non-paraffinic alternative jet fuels, such as those produced by hydroprocessed depolymerized cellulosic jet (e.g. KiOR) or catalytic hydrothermal (e.g. Readijet) processes which have been tested as part of the CLEEN program. These processes generate alternative fuels with distributions of aromatic species that are different from those found in conventional jet fuel, and consequently demonstrate different emissions behavior.

Research Approach

Introduction

In the ASAF model, the soot formation rate is assumed to consist of two components: one proportional to the fuel aromatics content, and one independent of fuel aromatics. For fuels where the distribution of aromatic compounds differs from that found in conventional jet fuel, accounting for differences in soot-production efficacies among classes of aromatic compounds can improve the fidelity of the model. Our approach to this task was to examine how the chemical kinetics specific to different fuel components leads to differences in soot formation, and use this to determine how measured fuel properties can be to improve predictions of soot formation.

Fuel Compositions

Alternative fuel compositions can differ significantly from conventional jet fuel. Among the alternative fuels currently available FT, HEFA, and DSHC fuels consist mainly of iso- and n-paraffins. CH has distributions of aromatic compounds similar to Jet A. HDCJ has large fractions of dicycloparaffins and indans/tetralins. Each of these fuel components can have a distinct contribution to the nvPM emissions performance of an alternative jet fuel. Typical compositions for alternative jet fuels, compared with conventional jet fuel, are show in Figure 3.

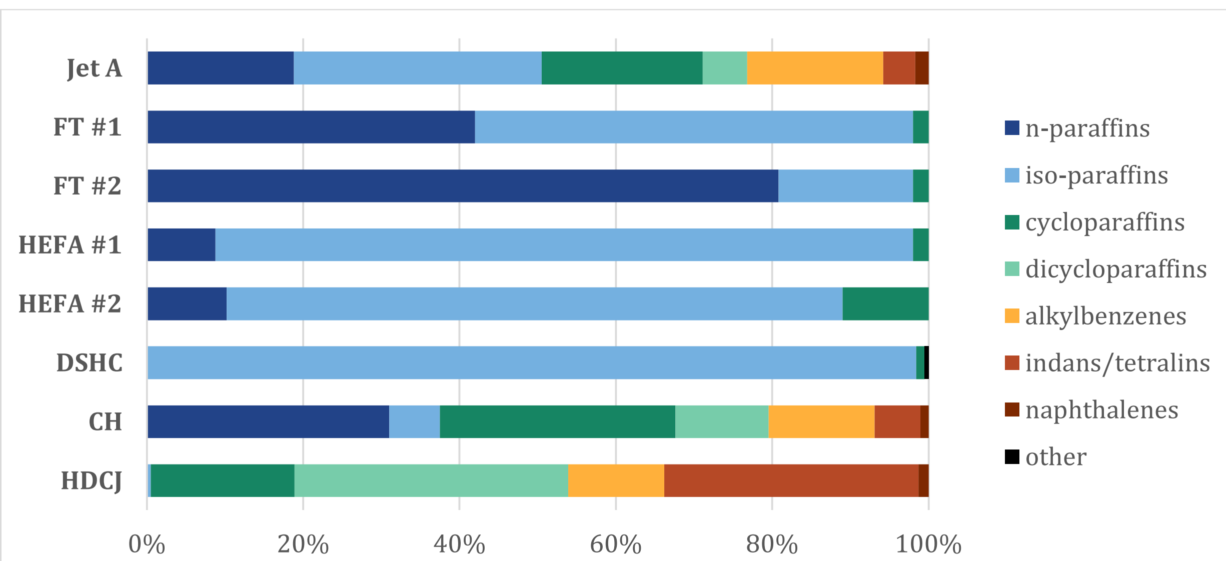

Figure 3: Typical chemical compositions of conventional and alternative jet fuels.

Threshold Sooting Index

One measure of a fuel's propensity to generate soot is the threshold sooting index (TSI), which is a property that can be measured in lab-scale diffusion flames (Olson and Pickens, 1984; Watson et al., 2013). TSI values for a wide range of hydrocarbon compounds have been tabulated in the literature (REFS). The TSI is a normalized measure of the sooting propensity of a fuel, with a high sooting fuel (naphthalene) assigned a TSI of 100 and a low sooting fuel (ethane) assigned a TSI of zero. The TSI of a fuel species depends on its structure and composition. TSI values from a range of fuel components are shown in Figure 4.

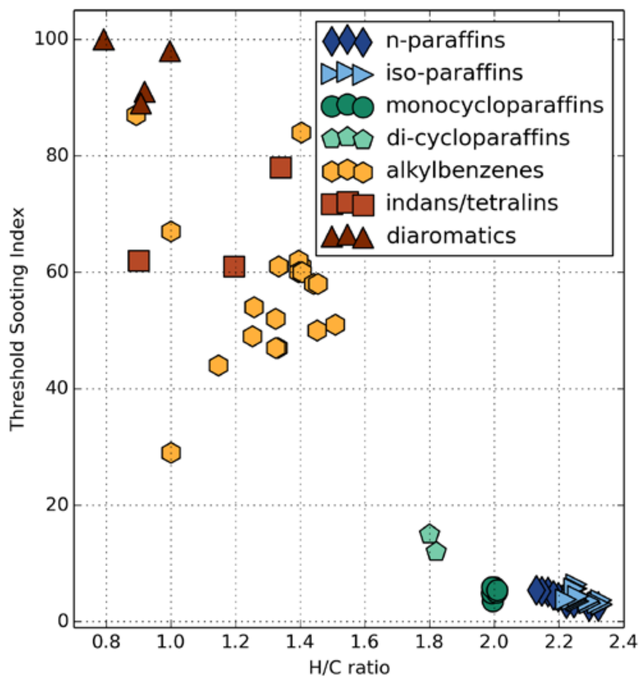

Figure 4: Threshold sooting index (TSI) for representative fuel species, classified by molecular structure.

While the TSI is partially correlated to H/C ratio, there is high variability among aromatic fuel components with similar H/C ratios. Estimating nvPM emissions indices from the TSI requires additional modeling. The TSI is determined only at one condition, and therefore does not provide information on what changes may occur as operating conditions such as temperature, pressure, or equivalence ratio change. For this, we utilize the reactor network model that was described under Task 2.

Reactor Modeling
We utilize the reactor network described under Task 2 to examine the trends in emissions between different fuel components as a function of engine and combustor conditions. The variation in nvPM emissions with fuel type shows the expected trends among molecular families, with high nvPM emissions from tetralins, lower from single-ring aromatics, lower still from cyclo-paraffins, and lowest from normal and iso-paraffins. These trends qualitatively follow the trends observed in the TSI measurements.

In addition, the nvPM emissions depend strongly on equivalence ratio, an effect which is not explicitly captured by TSI. Differences between molecular families diminishes at higher equivalence ratios, consistent with the observed behavior for alternative fuels, where the differences between conventional and alternative fuels decrease at high thrust settings where the fuel flow rates are highest and there are likely to be more regions of high equivalence ratio in the combustor.

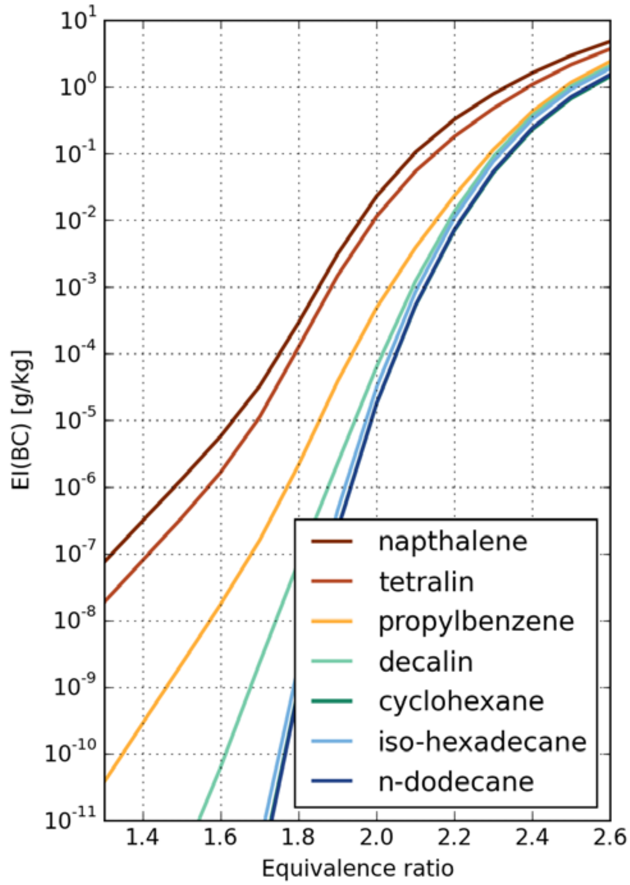

Figure 5: nvPM emissions indices for representative jet fuel components as a function of equivalence ratio.

Milestone(s)

Milestone 3: Prepare a paper for journal publication describing the improved nvPM model. Preparatory steps have been taken toward producing a paper, but completion of this milestone is contingent on the availability of the cruise-altitude alternative fuels emissions data which has not yet been released.

Major Accomplishments

Using reactor network simulations, we have demonstrated that detailed chemical kinetic models are able to capture differences in BC formation between different fuel species and among different families of chemical compounds which can be identified by detailed fuel analyses (e.g. GCxGC).

Outreach Efforts

A presentation describing the analysis of altitude and fuel composition effects using the reactor network model was given in the AEC Roadmap Teleconference on September 24, 2015.

References

Döpelheuer, A., Lecht, M., 1999. Influence of engine performance on emission characteristics, in: RTO Meeting Proceedings. Presented at the RTO AVT Symposium on Gas Turbine Engine Combustion Emissions and Alternative Fuels, Lisbon, Portugal.

Olson, D.B., Pickens, J.C., 1984. The effects of molecular structure on soot formation, I. Soot thresholds in premixed flames. Combustion and Flame 57, 199–208.

Ranzi, E., Frassoldati, A., Grana, R., Cuoci, A., Faravelli, T., Kelley, A.P., Law, C.K., 2012. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. Progress in Energy and Combustion Science 38, 468–501.

Speth, R.L., Rojo, C., Malina, R., Barrett, S.R.H., 2015. Black carbon emissions reductions from combustion of alternative jet fuels. Atmospheric Environment 105, 37–42.

Stettler, M.E.J., Boies, A.M., Petzold, A., Barrett, S.R.H., 2013. Global Civil Aviation Black Carbon Emissions. Environ. Sci. Technol. 47, 10397–10404.

Watson, R.J., Botero, M.L., Ness, C.J., Morgan, N.M., Kraft, M., 2013. An improved methodology for determining threshold sooting indices from smoke point lamps. Fuel 111, 120–130.