Project 039 Naphthalene Removal Assessment

Massachusetts Institute of Technology

Project Lead Investigator

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- P.I.(s): Prof. Steven Barrett & Dr. Raymond Speth
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- Period of Performance: July 8, 2016 to Aug. 31, 2020 (With the exception of funding and cost share information, this report covers the period from October 1st, 2017 to September 30th, 2018)
- Task(s):
    1. Estimate capital and operating costs of naphthalene removal
    2. Explore relationship between PAH formation and aircraft PM emissions
    3. Compare kinetic model results to LFP/PIMS experimental data
    4. Calculate air quality and climate impacts of naphthalene removal
    5. Conduct integrated cost-benefit analysis of impacts of naphthalene removal in the U.S.

Project Funding Level

Project Funding Level: $490,000 FAA funding and $490,000 matching funds. Sources of match are approximately $129,000 from MIT, plus 3rd party in-kind contributions of $361,000 from Oliver Wyman Group.

Investigation Team

Prof. Steven Barrett (MIT) serves as principal investigator for the A39 project as head for the Laboratory for Aviation and the Environment. Prof. Barrett coordinates both internal research efforts and maintains communication between investigators in the various MIT research teams mentioned below.

Dr. Raymond Speth (MIT) serves as co-principal investigator for the A39 project. Dr. Speth directly advises student research in the Laboratory for Aviation and the Environment focused on assessment of naphthalene removal refinery options, climate and air quality modelling, and fuel alteration life-cycle analysis. Dr. Speth also coordinates communication with FAA counterparts.

Prof. William Green (MIT) serves as a co-investigator for the A39 project as a head of the Green Research Group. Prof. Green advises student work in the Green Research Group focused on computer-aided chemical kinetic modeling of PAH formation.

Mr. Randall Field (MIT) is the Executive Director of the MIT Energy Initiative, and a co-investigator of the A39 project. Drawing upon his experiences as a business consulting director at Aspen Technology Inc., Mr. Randall provides mentorship to student researchers in selection and assessment of naphthalene removal refining option, and process engineering at-large.

Mr. Drew Weibel (MIT) is a graduate student researcher in the Laboratory for Aviation and the Environment. Mr. Weibel is responsible for conducting selection and assessment of naphthalene removal refining options, calculation of refinery process requirements and fuel composition effects from selected processes, relating PAH formation to aircraft PM emissions, estimating capital and operating costs of naphthalene removal, air quality and climate modelling, and an integrated cost-benefit analysis.

Mr. Max Liu (MIT) is a Ph.D. candidate in the Green Research Group. Mr. Liu is responsible for development and analysis of a chemical kinetic model of PAH formation with fuel-composition effects.

Dr. Mica Smith (MIT) is a Postdoctoral associate in the Green Research Group. Ms. Smith is responsible for the experimental measurements which are being used for the validation of the chemical kinetic mechanisms.

Dr. Agnes Jocher (MIT) is a Postdoctoral associate in the Green Research Group. Ms. Jocher is responsible for evaluating microphysical models which link the presence of PAH molecules to the formation of soot particles and providing modeling expertise on combining these models with the kinetic models being developed.

Project Overview

Aircraft emissions impact the environment by perturbing the climate and reducing air quality, which leads to adverse health impacts, including increased risk of premature mortality. As a result, understanding how different fuel components can influence pollutant emissions, as well as the resulting impacts and damages to human health and the environment, is of importance to leading future research aims and policy. Recent emissions measurements have shown that removal of naphthalenes, while keeping total aromatic content unchanged, can dramatically reduce emissions of particulate matter (Brem *et al* 2015, Moore *et al* 2015). The objective of this research is to determine the benefits, costs, and feasibility of removing naphthalenes from jet fuel, in regards to the refiner, the public, air quality, and the environment. Specific goals of this research include:

- Assessment and selection of candidate refining processes for the removal of naphthalenes from conventional jet fuel, including details of required technology, steady-state public cost, and changing life-cycle emissions impacts at the refinery.
- Development of a chemical kinetics model to better understand the link between fuel aromatic composition resulting PM emissions due to jet fuel combustion.
- Assessment of the intrinsic climate and air quality impacts associated with naphthalene reduction and/or removal from jet fuel.
- Development of a succinct life-cycle analysis of the relative costs of removing naphthalene from jet fuel and the associated benefits due to avoided premature mortalities and climate damages for a range of possible scenarios.

Task 1- Estimate Capital and Operating Costs of Naphthalene Removal

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Objective(s)

The objective of this task is to evaluate refinery technologies which can be used to remove naphthalene to determine their feasibility, costs, and effects on fuel composition. This includes calculating the costs of constructing new refinery unit processes, and determining additional utility and other operating costs associated with operating the process units responsible for naphthalene removal.

Research Approach

Naphthalene is present in varying levels in the straight-run crude oil distillation cuts used to produce jet fuel. For cuts which exceed the 3% volume limit on naphthalenes (ASTM D1655 2016), this exceedance can be resolved solely through blending, since the average naphthalene content of commercial Jet A is ~1.4% (DLA Energy 2013). Reducing the naphthalene content of jet fuel or eliminating it would therefore require the introduction of additional refinery processing. After reviewing several candidate refining processes in the previous year of this project, we have decided to further explore two in detail: selective hydrotreatment and extractive distillation. These processes are both used in industry for reduction or separation of aromatics and show promise in their ability to reduce and remove naphthalene from jet fuel. Selective hydrotreatment reacts hydrogen with the feedstock and leads to removal of impurities and saturation of aromatics. Extractive distillation allows for the full separation of aromatics from the feedstock via polar solvents. The aromatics stream can then be processed to separate mono-aromatics and naphthalenes, with the former stream being returned to the jet fuel blending pool. These processes were chosen for their low added complexity and energy and because they have a minimal effect on the resultant fuel properties. It is, however, important to note that changes in fuel density, specific energy, fuel sulfur content, hydrogen content, and aromatic content will occur and are considered.

We have developed fundamental process models to estimate effects of fuel constituents and completed a literature search to collect data on process energy requirements, capital costs, and operating costs for both hydro-treatment and extractive distillation. In order to evaluate each candidate process, we leverage existing literature to estimate the utility (process fuel, electricity, hydrogen, etc.) requirements for each process, the effect on the composition of the resulting jet fuel, and the capital costs of new refinery equipment required, including the effects and costs of pre-processing and auxiliary process units that may be required. We then compare processes side-by-side in order to demonstrate the trade-offs associated with naphthalene removal at the refinery.

We consider the hypothetical adoption of a policy whereby jet fuel naphthalene content in the U.S. is reduced by 95% via either hydro-treatment or extractive distillation, at each of the 116 operational U.S. refineries with capacity of greater than 1000 barrels per day (BPD). We calculate costs using a stochastic discounted cash flow model of each refinery. Refinery capital costs are calculated using standard cost curve estimation methods, which relate process unit costs to capacity. Cost curves are used for both the primary naphthalene-removing process units (e.g. extractive distillation column or hydrotreater) as well as auxiliary process units (e.g. steam-methane reformer, CLAUS sulfur recovery unit, pressure-swing hydrogen recovery units, and steam generators). Direct operating costs include maintenance, local taxes, insurance, and supplies, calculated as a percentage of capital costs. Variable operating costs such as process water and chemicals are calculated based on the process unit utility requirements. The stochastic refinery model is used to determine the net present value (NPV) of each naphthalene removal process over its operating lifetime. The NPV can also be used to calculate the cost premium (i.e. cents per gallon) associated with the production of naphthalene-free fuel. Cost estimates are considered from two perspectives: that of the fuel market, and that of society. The market perspective computes cost premiums including all cash flows incurred by fuel producers, thus estimating the expected increase in the market price for naphthalene-free jet fuel. The societal cost estimate is computed from a resource-based perspective, placing it on the same basis as the monetization of potential benefits from improved air quality and potential climate impacts. In this perspective, redistribution of resources, e.g. taxes or loan payments, are disregarded, and the discount rate is assumed to be equivalent to society’s long-term cost of capital.

Milestone(s)

The work completed for this task was documented in Deliverable 2-1, provided to the FAA on November 30, 2017.

Major Accomplishments

The resource-based (societal) cost premium and market cost premium estimate distributions for a policy in which all US produced jet fuel has its naphthalene content reduced by 95% (to 0.06 vol%) are shown in **Figure 1**, with cost data presented in 2016 USD. The mean societal cost premium of hydro-treating is found to be 2.4 cents/liter (95% confidence interval (CI): 2.3–2.5) and of extractive distillation is 1.7 cents/liter (95% CI: 1.6–1.8). This represents an annual NPV of $2.26 billion/year (95% CI: 2.17–2.35) and $1.65 billion/year (95% CI: 1.58–1.73), respectively.

The mean market cost premium of hydro-treating is 4.7 cents/liter (95% CI: 4.6–4.8) and of extractive distillation is 3.1 cents/liter (95% CI: 3.0–3.2). Given the average US Gulf Coast cost of jet fuel in 2016 was $0.33/liter, this represents a 14% and 9% increase in the cost of jet fuel for naphthalene removal via hydro-treatment and extractive distillation, respectively.

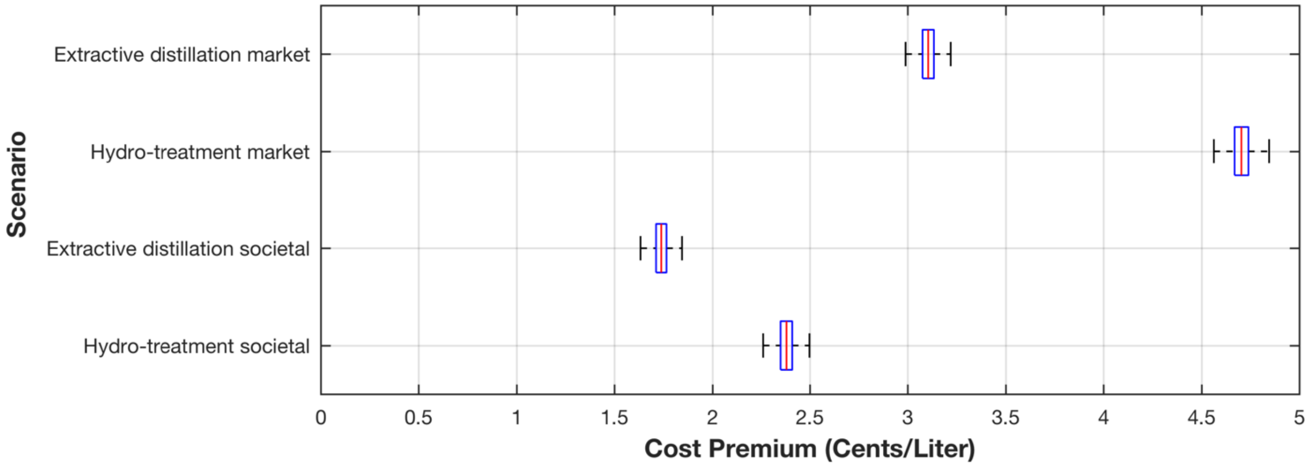

Figure 1. Boxplot for the societal and market cost premiums of hydro-treatment and extractive distillation. All values provided in cents/liter. Red markers represent the distribution means, blue boxes represents the first and third quartiles, and whiskers represent the 95% confidence interval.

Publications

This work is currently being prepared for publication as a paper entitled "Techno-economic Assessment of Removing Jet Fuel Naphthalene to Reduce Aviation-attributable Non-volatile Particulate Matter Emissions."

Outreach Efforts

Drew Weibel gave a presentation entitled "Naphthalene Removal Assessment: Cleaning up Jet Fuel for Reduced Environmental Impacts" at the CRC Aviation Meeting on May 3, 2018.

Student Involvement

This task was conducted primarily by Drew Weibel, working directly with Prof. Steven Barrett and Dr. Raymond Speth.

Plans for Next Period

This task has been completed.

Task 2- Explore Relationship Between PAH Formation and Aircraft PM Emissions

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Objective(s)

The formation of black carbon (soot) from hydrocarbon fuels can be considered as taking place in two stages. First, fuel components and combustion intermediates react to form polycyclic aromatic hydrocarbons (PAHs). Large PAHs then act as soot nuclei, which grow as they absorb both PAH and other species, coagulate through collisions with other soot particles, carbonize, and partially oxidize (Richter and Howard 2000). The details of fuel composition mainly affect the first step of this process, the formation of PAHs. The objective of this task is to develop chemical kinetic mechanisms and combustor models which include the formation of PAH species from different fuel components and the conversion of these PAH species to soot particles (or nvPM emissions), in order to be able to evaluate the sensitivity of nvPM emissions to fuel composition.

Research Approach

The Reaction Mechanism Generator (RMG) was used to develop a detailed chemical kinetic mechanism for jet fuel combustion that includes the formation of PAH (Gao *et al* 2016). As part of this task, we have extended RMG to include recently-discovered PAH growth pathways, such as the phenyl addition pathway, cyclization via carbenes, and an aromatic-catalyzed intramolecular H-transfer mechanism. We then used this improved version of RMG to generate a higher-fidelity chemical kinetic model for the formation of PAHs in naphthalene-containing flames. This approach is being utilized to produce a chemical kinetic mechanism describing the first stage of soot particle production.

These mechanisms are then utilized within Cantera (Goodwin *et al* 2013), a combustion modelling framework, to compute PAH formation rates in fundamental combustion configurations. A schematic of the combustor model with the soot microphysical model is shown in Figure 2.

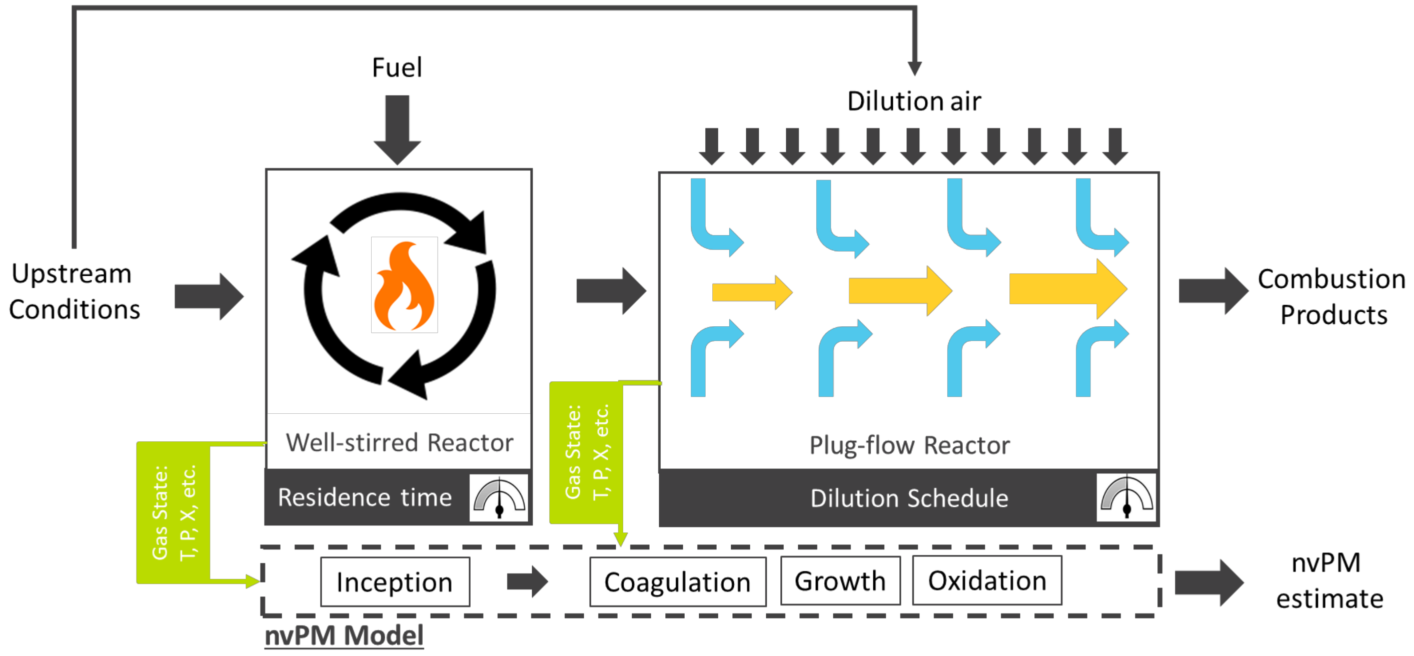

Figure 2. Schematic of a gas turbine combustor model including nvPM microphysical model

The second stage of soot formation is less well understood and more dependent on conditions within the combustor, such as fuel atomization and local temperature and pressure. In order to both capture differences between engines and avoid the uncertainties of modeling soot nucleation and growth processes, we have utilized existing analyses of PM emissions from aircraft engines to develop bounding scenarios describing the extent to which naphthalene removal results in decreases in expected PM emissions.

Milestone(s)

The work completed for this task was documented in Deliverable 2-2, provided to the FAA on February 28, 2018.

Major Accomplishments

The chemical kinetic mechanism and combustor model developed were used to calculate formation rates of PAH species over a range of engine relevant conditions. Figure 3 shows the evolution of several key aromatic species as the engine thrust setting is varied from near-idle to full power conditions for a representative surrogate fuel.

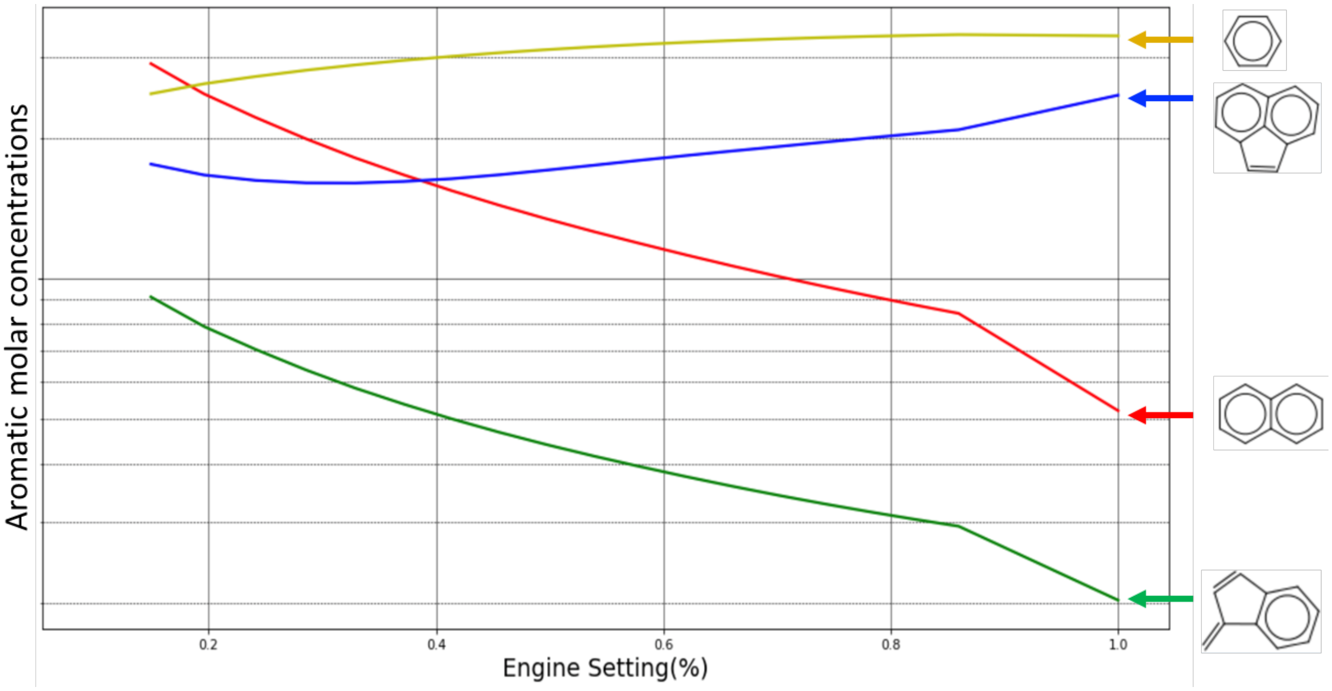

Figure 3. Evolution of selected aromatic species concentrations in the combustor primary zone as a function of engine setting.

Outreach Efforts

Raymond Speth gave a presentation with an overview of the project at the Aviation Emissions Characterization Roadmap Meeting on May 23, 2018.

Student Involvement

This task was conducted primarily by Drew Weibel, working directly with Prof. Steven Barrett and Dr. Raymond Speth.

Plans for Next Period

This task has been completed.

Task 3- Compare Kinetic Model Results to LFP/PIMS Experimental Data

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Objective(s)

The growth of aromatic rings as part of PAH formation is controlled by radical reactions, especially the hydrogen abstraction – C_2H_2 addition (HACA) mechanism. The objective of this task is to produce experimental data which can be used to improve estimates of rate coefficients used in chemical kinetic models of PAH formation.

Research Approach

Laser flash-photolysis photoionization mass spectrometry (LFP/PIMS) is an experimental technique in which a photolysis laser pulse initiates controllable, quantifiable radicals in a temperature and pressure controlled reactor. The evolution of the chemical composition in the reactor is then monitored by ionization with VUV light and detection with a mass spectrometer. Experimental conditions are simulated using reactor modeling software, using rate coefficients estimated from the literature. Because these rate coefficients are often pressure dependent, quantum chemistry calculations are used to extrapolate from the low-pressure experimental values to the high pressures relevant to engine operations. Simulations using RMG-generated mechanisms are compared with literature-based rates and the experimental results in order to improve important pathway parameters for aromatic growth.

For this task, two pathways were evaluated. The first is the addition of a vinyl radical (C_2H_3) to acetylene (C_2H_2), which is key step in a formation pathway for benzene (C_6H_6). Studying this system allows us to confirm that we can observe ring formation in our experiment, and measure the kinetics and branching ratios which describe C_4H_5/C_4H_4 formation and the yield of benzene, as shown in Figure 4.

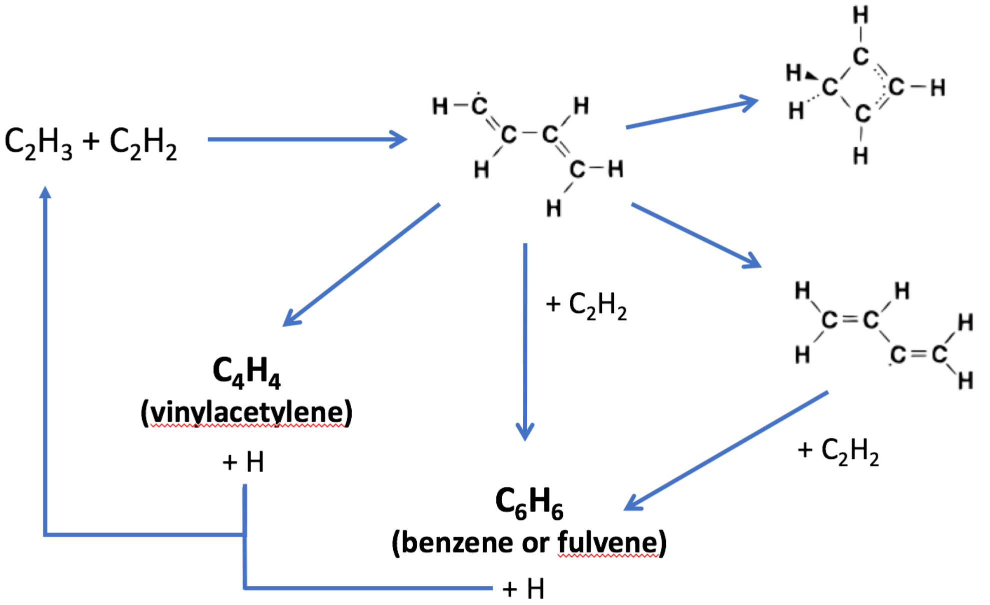

Figure 4. Formation pathways of benzene from vinyl radical and acetylene

The second pathway which was explored is acetylene addition to naphthyl radicals. While aromatic growth from naphthalene is thought to be dominate by the HACA mechanism, under experimental conditions, three-ring PAHs have generally not been observed. This leads to the question of what other pathways could exist that convert naphthalenes to PAHs, which can be explored using LFP-PIMS.

Milestone(s)

The work completed for this task was documented in Deliverable 2-3, provided to the FAA on April 30, 2018.

Major Accomplishments

Results for the vinyl radical – acetylene pathway, comparing experimental time profiles with simulations, are shown in Figure 5. Kinetics calculated from LFP-PIMS were found to generally agree with the results of the RMG-generated model over a range of temperatures. Preliminary experiments for 1-naphthyl addition to C_2H_2 revealed branching between stable $C_{12}H_8$ products (e.g. acenaphthalene) and $C_{12}H_9$ adducts, as shown in Figure 6. Work is ongoing to incorporate this finding into RMG.

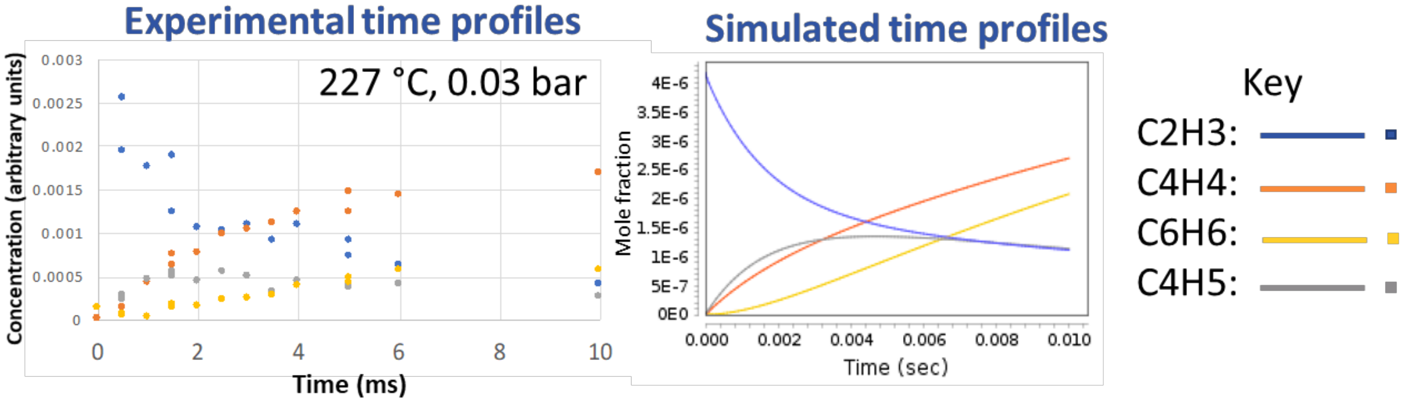

Figure 5. Comparison of experimental and simulated concentration profiles for reaction of vinyl radical and acetylene.

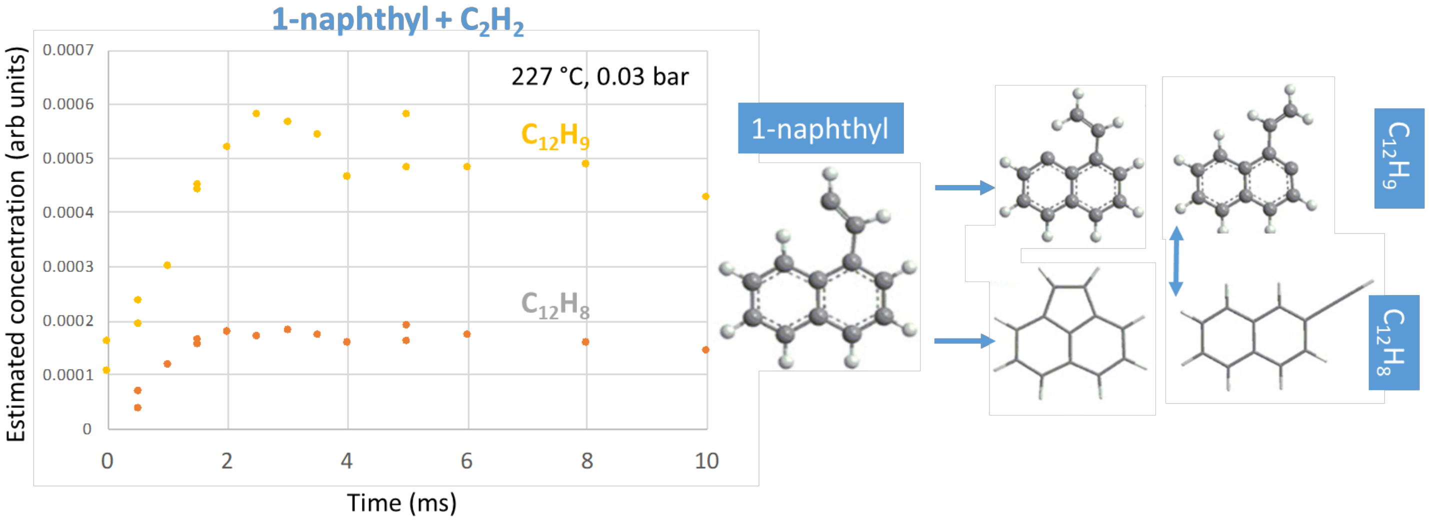

Figure 6. Experimentally-observed branching ratios between stable $C_{12}H_8$ species and $C_{12}H_9$ adducts formed by the reaction of 1-naphthyl radicals with acetylene.

Student Involvement

This work was conducted primarily by Dr. Mica Smith, a postdoctoral associate working under the supervision of Prof. William Green.

Plans for Next Period

This task has been completed.

Task 4- Calculate Air Quality and Climate Impacts of Naphthalene Removal

Massachusetts Institute of Technology

Objective(s)

The objective of this task is to calculate the air quality and climate impacts of a policy in which naphthalene is removed from jet fuel used in the United States.

Research Approach

The air quality effects of changes in aircraft PM emissions are evaluated using the GEOS-Chem adjoint model, which we have previously used for assessing health impacts of emissions (Dedoussi and Barrett 2014). The use of an adjoint model, which is a computationally-efficient approach to calculating sensitivities of an aggregate objective function (e.g. population exposure to $PM_{2.5}$), makes it possible to evaluate a range of scenarios in a single run, which allows incorporation of upstream uncertainty in the emissions indices for different species. The PM exposure calculated using GEOS-Chem includes both the effects of changes in black carbon emissions and changes due to sulfur reductions which accompany the removal of naphthalenes (in the case where hydrotreating is used to remove naphthalenes). The spatial pattern of emissions of nvPM, and sulfur compounds is taken from the 2015 inventory from the Aviation Environmental Design Tool (AEDT).

Climate impacts of naphthalene removal include contributions both at the fuel production and fuel consumption stages. The additional refinery processing required to reduce or remove naphthalene requires process fuel, steam, electricity, and, in the case of hydrotreating, hydrogen production. The greenhouse gas (GHG) emissions associated with each of these processes increase lifecycle jet fuel GHG emissions. Using the results calculated in Task 1, the GHG emissions associated with naphthalene removal were found to be 135 g CO_2e per kg fuel for hydro-treating and 144 g CO_2e per kg fuel for extractive distillation. Consumption of reduced-naphthalene fuel decreases radiative forcing from aviation black carbon, while reductions in sulfur reduce the cooling effect of sulfates (Mahashabde *et al* 2011). The combined climate impacts of these effects are evaluated using the APMT-Impacts Climate model, which is a policy-oriented rapid assessment tool that provides probabilistic estimates of climate impacts.

Milestone(s)

The work completed for this task was documented in Deliverable 2-4, provided to the FAA on May 31, 2018.

Major Accomplishments

Based on a literature review of nvPM emissions measurements from engines using fuels with varying levels of naphthalene (DeWitt *et al* 2008, Brem *et al* 2015), the potential range of reduction in nvPM emissions associated with 95% naphthalene removal was estimated to be 15–40%, or 5.0–12.5 mg nvPM per kg fuel. Monetized climate impacts for the different climate forcing pathways are summarized in Table 1, presented on a cents per gallon basis with both median values and a range indicating the 90% confidence interval. Monetized air quality impacts of naphthalene removal are similarly summarized in Table 2.

Table 1. Monetized climate benefits of naphthalene removal

Impact Pathway	Impact (¢/gallon)
BC radiative forcing (15% nvPM reduction)	0.09 (90% CI: 0.01 – 0.23)
BC radiative forcing (40% nvPM reduction)	0.23 (90% CI: 0.04 – 0.61)
Hydrotreating CO_2 emissions	-1.82 (90% CI: -0.30 – -4.70)
Extractive distillation CO_2 emissions	-1.89 (90% CI: -0.31 – -5.01)
Sulfate aerosol (hydrotreating only)	-4.17 (90% CI: -0.61 – -11.23)

Table 2. Monetized air quality benefits of naphthalene removal

Impact Pathway	Impact (¢/gallon)
nvPM emissions (15% nvPM reduction)	0.04 (90% CI: 0.02 – 0.06)
nvPM emissions (40% nvPM reduction)	0.11 (90% CI: 0.06 – 0.16)
Sulfur emissions (hydrotreating only)	1.92 (90% CI: 1.04 – 2.76)

Student Involvement

This task was conducted primarily by Drew Weibel, working directly with Prof. Steven Barrett and Dr. Raymond Speth.

Plans for Next Period

This task has been completed as originally planned. The current results do not include the effect that changes in nvPM emissions have on contrails, which are a significant component of aviation's climate impact. As such, additional work has been planned to estimate changes in contrail radiative forcing associated with the use of naphthalene-depleted fuels using the Contrail Evolution and Radiation Model (Caiazzo *et al* 2017). In addition, the air quality results are based on a regional atmospheric model, simulated at a resolution of 0.5° × 0.667°, while nvPM impacts have been shown to be underestimated with lower-resolution models (Punger and West 2013). Additional work has been planned to provide better estimates of these impacts based on higher-resolution local modeling approaches.

Task 5- Conduct Integrated Cost-benefit Analysis of Impacts of Naphthalene Removal in the U.S.

Massachusetts Institute of Technology

Objective(s)

The objective of this task is to produce an integrated cost-benefit analysis of naphthalene removal in the United States, accounting for the additional refining cost as well as the air quality and climate impacts.

Research Approach

The overall cost benefit assessment of naphthalene removal includes fuel production costs, air quality benefits, and climate impacts from fuel production and fuel consumption. These effects are placed on a common monetized basis in order to compare different naphthalene removal scenarios. We consider uncertainties in the assessment of each component and use these uncertainties to compute the likelihood of a net benefit for different scenarios.

Milestone(s)

The work completed for this task was documented in Deliverable 2-5, provided to the FAA on July 31, 2018.

Major Accomplishments

The processing costs, air quality benefits, and climate impacts of naphthalene removal are converted to a common basis of cents per gallon, and presented in Table 3. The totals shown exclude contrail effects, which have not yet been quantified. In the absence of large impacts on contrail net radiative forcing, the current results suggest that the benefits of widespread naphthalene removal are outweighed by the costs of processing the fuel and the CO$_2$ emissions associated with that processing.

Table 3. Costs (positive) and benefits (negative) of naphthalene removal.

	Component	Hydrotreatment (¢/gallon)		Extractive Distillation (¢/gallon)	
Air quality	nvPM	-0.1	(-0.02 – -0.16)	-0.1	(-0.02 – -0.16)
	Fuel sulfur	-1.9	(-1.1 – -2.7)	0	
Climate	nvPM	-0.2	(-0.02 – -0.6)	-0.2	(-0.02 – -0.6)
	Fuel sulfur	4.1	(0.6 – 11.1)	0	
	Contrails	*unknown*		*unknown*	
	Refinery CO$_2$	1.9	(0.3 – 4.8)	1.9	(0.3 – 5.1)
Processing	Refinery	9.1	(8.7 – 9.5)	6.4	(6.1 – 6.8)
Total		**13.0**	**(9.0 – 20.7)**	**8.1**	**(6.5 – 11.4)**

For both naphthalene removal processes, the climate impacts of the refinery CO$_2$ emissions exceed the air quality and climate benefits of naphthalene removal, neglecting the potential for significant contrail effects. In addition, in the case of hydrotreatment, the net present value of the climate warming associated with sulfur removal is larger than the NPV of the reduced air-quality related damages. In addition to these environmental costs are the costs associated with processing jet fuel in the refinery. These results suggest that, in the absence of a strong contrail effect, it is unlikely that naphthalene removal on a nationwide basis would be cost beneficial. However, naphthalene removal may still be beneficial under certain circumstances, e.g. if applied to fuels used at airports with particular air quality concerns.

Student Involvement

This task was conducted primarily by Drew Weibel, working directly with Prof. Steven Barrett and Dr. Raymond Speth.

Plans for Next Period

This task, as originally planned, has been completed. Future work includes incorporating estimates of the effect of naphthalene on contrail climate impacts, as well as the potential to evaluate scenarios where naphthalene is removed only at certain places or times in order to maximize the benefit, e.g. targeting fuel used at specific airports.

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