Project 039 Naphthalene Removal Assessment

Massachusetts Institute of Technology

Project Lead Investigator

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University Participants

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- P.I.: Prof. Steven Barrett
- Co-PI: Dr. Raymond Speth
- FAA Award Number: 13-C-AJFE-MIT, Amendment No. 026
- Period of Performance: July 8, 2016 to Aug. 31, 2017 (reporting with the exception of funding levels and cost share only for the period from July 8 1, 2016 to September 30, 2016).
- Task:
    1. Preliminary screening of refinery processes for naphthalene removal

Project Funding Level

$200,000 FAA funding and $200,000 matching funds. Sources of match are approximately $52,000 from MIT, plus 3rd party in-kind contributions of $148,000 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. Field 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 researcher 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 and developing a relationship between PAH formation and aircraft PM emissions.

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. 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 costs to the refiner and the public, 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: Preliminary Screening of Naphthalene Removal Refining Processes

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Objective(s)

Naphthalene is present in varying levels in straight-run crude oil distillation cuts used to produce jet fuel, and is currently not targeted for removal in treatments used to meet industry standards. As a result, reducing the naphthalene content in jet fuel entails the introduction of an additional refinery treatment process. The objective of this task is to identify suitable refinery processes that can be used to remove or convert naphthalenes. Once identified, the process will be evaluated through analysis of the associated utility/feedstock inputs and costs of adding each treatment process to the refinery and running it at scale.

Research Approach

In order to screen potential refining processes to be used for naphthalene removal 1) a literature review will be conducted to identify candidate refining processes, 2) the candidate processes will be evaluated against each other, and 3) the trade-off associated with different levels of naphthalene removal will be assessed.

Literature Review

There are a number of processes which could potentially be employed to remove or convert naphthalene's, including selective hydrogenation, liquid-liquid extraction, adsorbents, and reactive distillation. By leveraging existing literature, potential naphthalene removal refining processes will be selected along with the level of technological innovation required (if any). Particular attention will be given to preserving non-naphthalenic aromatics, since reducing the amount of these components would limit the capacity to blend paraffinic alternative jet fuels while still meeting minimum requirements for aromatics.

Process Evaluation

In order to evaluate each candidate process, we will 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. We will include the effects of any pre-processing that may be required. We will then compare processes side in order to demonstrate the trade-offs associated with naphthalene removal at the refinery.

Removal Severity
As a by-product of analyzing a range of different refining pathways, we will be able to assess the tradeoffs associated with different levels of naphthalene removal. Combined with later work in development of a relationship between jet fuel composition and PAH formation, we will be able to assess the level of severity in which naphthalene's should be removed, in order to optimize costs and benefits.

Milestone(s)

Literature Review
A qualitative literature review was conducted to identify potential refining processes that can remove naphthalene from streams blended to produced jet fuel.

Major Accomplishments

Selection of Potential Naphthalene Removal Refining Processes
A set of candidate refining processes were chosen that could remove naphthalene from jet fuel intermediate streams. The chosen refining processes will be used throughout the remainder of the A39 project to determine the feasibility and associated utilities and costs of naphthalene removal.

Publications

None

Outreach Efforts

A poster describing the motivation and planned approach for this research was presented at the Fall ASCENT Meeting on September 27, 2016 in Washington, DC.

Awards

None

Student Involvement

Drew Weibel, a graduate student in the Laboratory for Aviation and the Environment is working directly with Prof Steven Barrett and Dr. Raymond Speth to conduct the research objectives of Task 1. Mr. Weibel is a 1st year graduate student, and will serve on the research team through the remainder of the A39 project timeline.

Plans for Next Period

Completion of Task 1
The remainder of Task 1 objectives will be met over next period of performance. The end product of task 1 will be the calculated process requirements and fuel composition effects of candidate naphthalene removal refining processes.

Future Work
In addition to Task 1, the effects of naphthalene content on the production of poly-aromatic hydrocarbon (PAH) molecules will be evaluated. A chemical kinetic model of PAH formation with included fuel-composition effects will be developed with Reaction Mechanism Generator (RMG) software. This model will be used along with Cantera, a combustion modeling framework, to compute PAH formation rates in fundamental combustion configurations. Along with existing aircraft engine PM emissions data, this platform will be used to develop scaling relations between PAH formation rates computed from the combustion model, and expected engine-specific PM emissions.