Project 39
Naphthalene Removal Assessment

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Motivation

- Aviation-attributable nvPM emissions (1) contribute to several cardiovascular and respiratory health issues, (2) result in a net positive radiative forcing (RF) through direct RF and by facilitating contrail (cirrus) formation, and (3) reduce the combustor service life[1][2]
- On average, naphthalenes (di-aromatic compound) make up only ~2 vol% of jet fuel[1]
- Naphthalenes in jet fuel are identified as disproportionate contributor to nvPM emissions, and complete removal of naphthalenes has been estimated to reduce nvPM number emissions by up to 70%[3]
- Jet fuel could be further processed at the refinery, via current finishing processes, to reduce or eliminate naphthalenes

Objectives

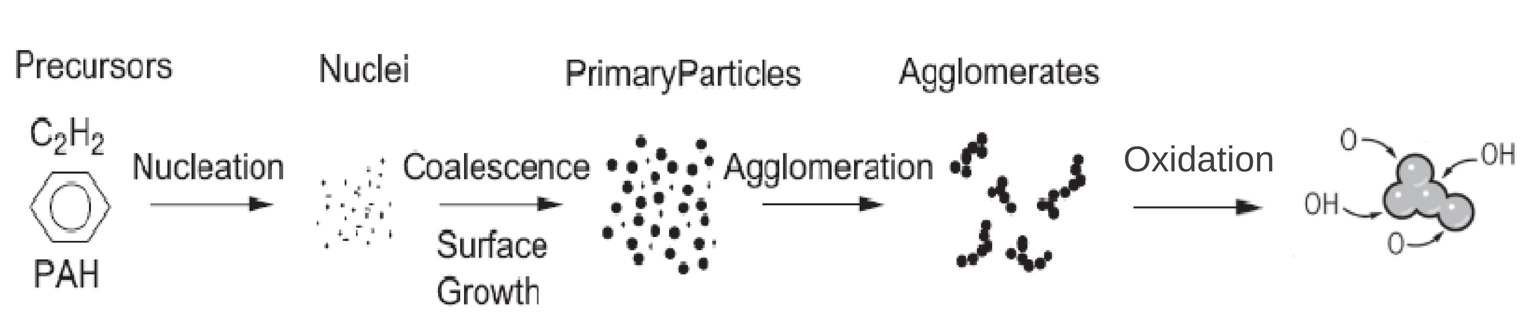
- Develop a combustor model able to predict nvPM emissions for different fuel compositions and for different phases of flight
- Conduct a comprehensive cost-benefit analysis of reduction or removal of naphthalene from U.S. produced jet fuel and its effect on aviation's air quality and climate impacts

nvPM Formation

Soot (nvPM) from turbine jet engines is composed of uniquely fine particles (10-60 nm in diameter) that form during incomplete combustion processes and consist of branched chains of near-spherical particles. The formation process happens in the order of milliseconds[4]. The overall process is complex, but can generally be divided into four main steps:

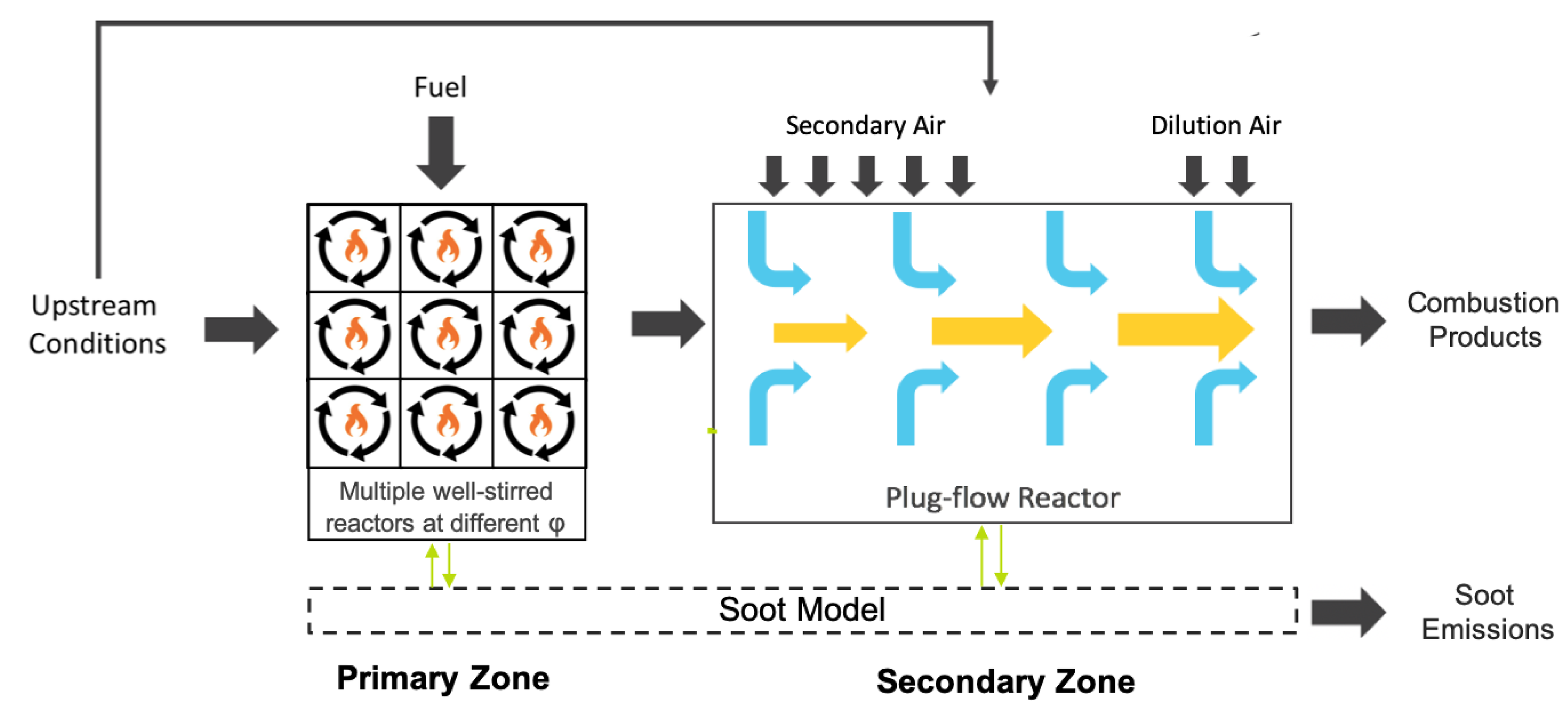
- Nucleation: Collisions of gaseous precursor species (PAHs) leads to the inception of solid soot particles
- Surface Growth: Soot particles grow by adsorption of gas phase molecules, primarily acetylene
- Coagulation: Soot particles grow further through particle-particle collisions
- Oxidation: Soot is destroyed during oxidation as carbon and hydrogen are removed from the soot agglomerates by reactions with oxygen and hydrogen

Mechanisms modeling these four steps are implemented and result in a computed soot number and mass density.



Combustor Model

The combustor model consists of a primary zone and a secondary zone. They are both coupled with a soot model, as schematically shown in the figure below.



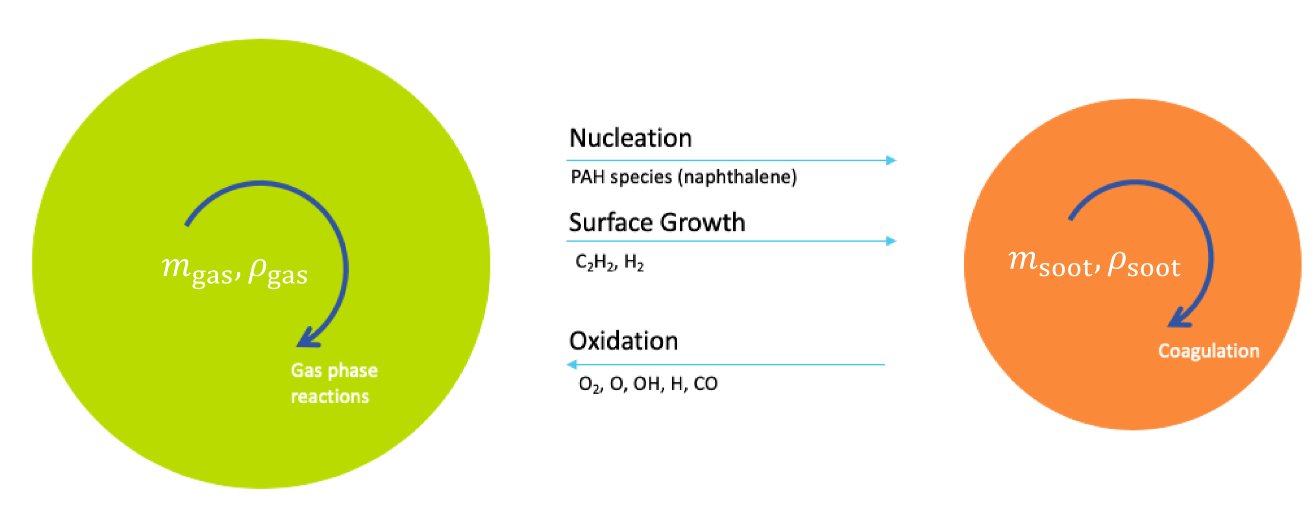
Primary Zone

- Upstream air is mixed with fuel and reacts with a certain characteristic residence time
- Modeled as *N* well-stirred ideal gas constant pressure reactors
- Using multiple reactors at different equivalence ratios allows for capturing the mixture inhomogeneity in the primary zone
- Equivalence ratios are normally distributed around mean with standard deviation dependent on the mixing parameter *S*[5]

Secondary Zone

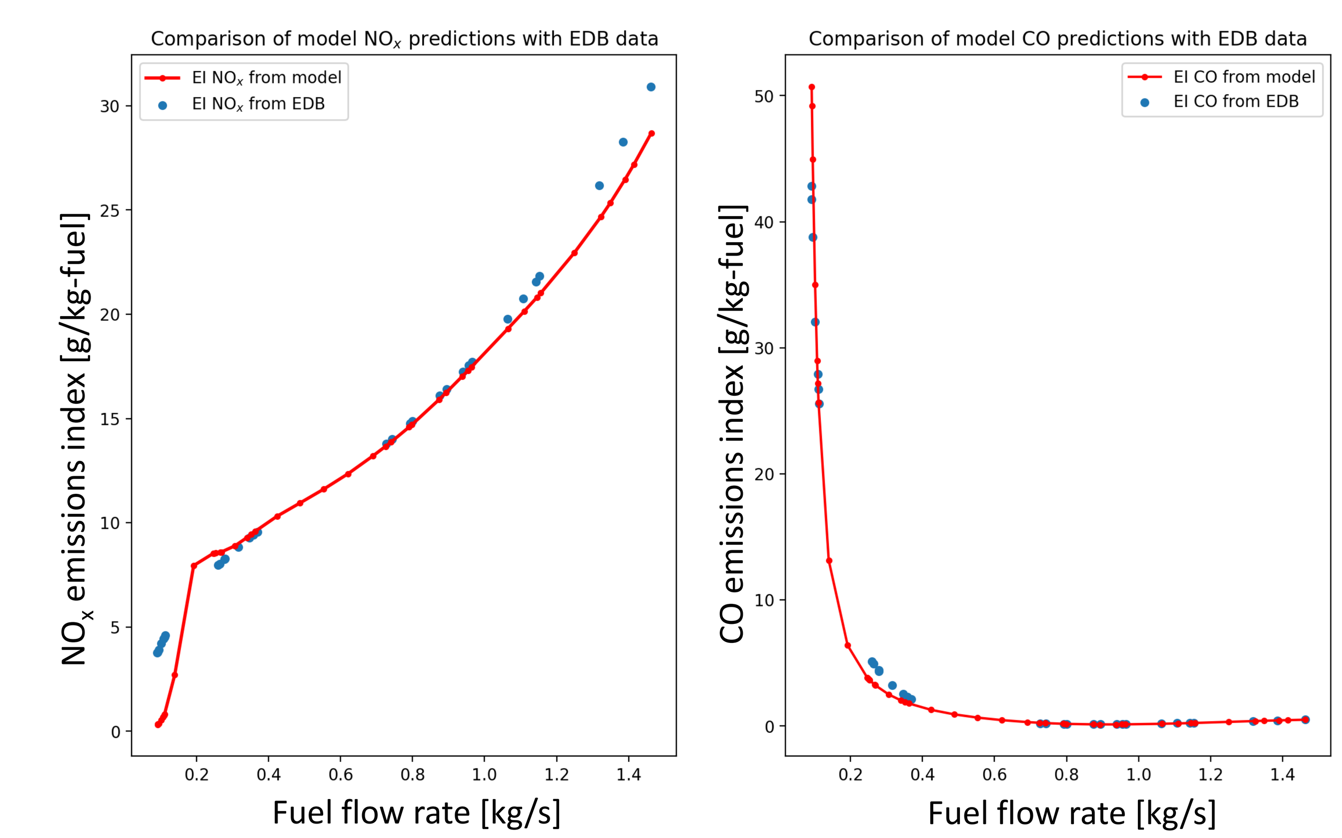
- Flow exiting the *N* primary zone reactors is mixed together upon entering the secondary zone
- Both secondary air and dilution air are added in the secondary zone
- Air insertion pattern found to strongly influence emission profiles, especially for rich primary zones[5]
- Secondary zone modeled as plug flow reactor

As soot forms and oxidizes, interactions between the gas phase and the solid soot phase take place. These phase interactions, illustrated in the figure below, are accounted for in the model by coupling soot formation and oxidation rates with rates of the gas phase reactions.



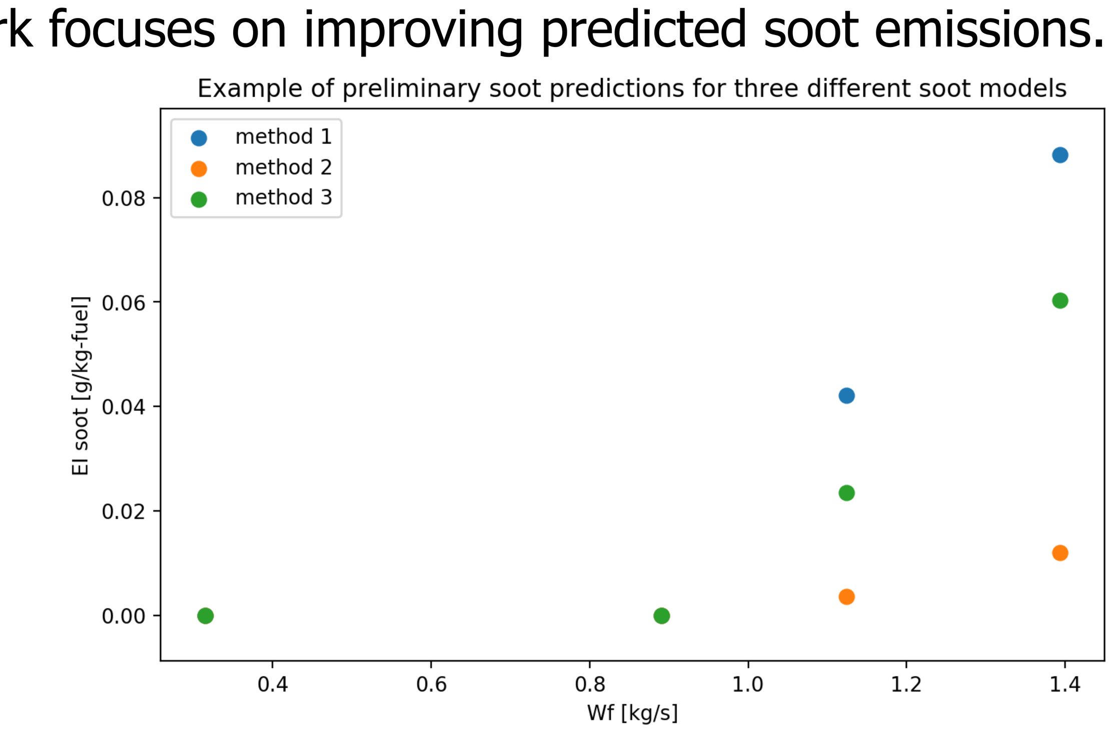
Model Optimization & Validation

Publically-available data from the EDB is used to determine model parameters that describe the combustor geometry and mixing characteristics and to validate the model. First, these parameters are optimized to match a subset of the data. Then, the model is run for the complete LTO cycle and the predictions are compared to the data. The parameter optimization can be repeated for different engine designs or when additional nvPM measurement data becomes available.



nvPM Mass Predictions

Initial results show expected trends and are found to be in the right order of magnitude. However, EIs at low thrust are underestimated. Current work focuses on improving predicted soot emissions.



Future Work

Calculate nvPM reductions associated with the use of naphthalene-free jet fuel and use this reduction to quantify air quality and climate benefits associated with naphthalene removal, including reductions in contrail radiative forcing. These benefits will then be monetized and compared to the previously-calculated costs of naphthalene removal.

Contributors & Collaborators

Prof. William Green, Randall Field, Drew Weibel, Mengjie Liu

References:

[1] B. T. Brem *et al.*, "Effects of Fuel Aromatic Content on Nonvolatile Particulate Emissions of an In-Production Aircraft Gas Turbine," *Environ. Sci. Technol.*, vol. 49, no. 22, pp. 13149–13157, Nov. 2015.

[2] H.T. Bocklehurst *et al.*, "Soot Predictions Within An Aero Gas Turbine Combustion Chamber," *International Gas Turbine & Aeroengine Congress & Exhibition,* June 1997.

[3] R. H. Moore *et al.*, "Influence of Jet Fuel Composition on Aircraft Engine Emissions: A Synthesis of Aerosol Emissions Data from the NASA APEX, AAFEX, and ACCESS Missions," *Energy Fuels*, vol. 29, no. 4, pp. 2591–2600, Apr. 2015.

[4] H. Omidvarborna *et al.*, "Recent Studies on Soot Modeling for Diesel Combustion," *Renewable and Sustainable Energy Reviews,* August 2015.

[5] J. B. Heywood *et al.*, "Parameters Controlling Nitric Oxide Emissions from Gas Turbine Combustors," *AGARD Propulsion and Energetics Panel 41st Meeting on Atmospheric Pollution by Aircraft,* April 1973.

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