FAA CENTER OF EXCELLENCE FOR ALTERNATIVE JET FUELS & ENVIRONMENT

Naphthalene Removal Assessment

Project 39

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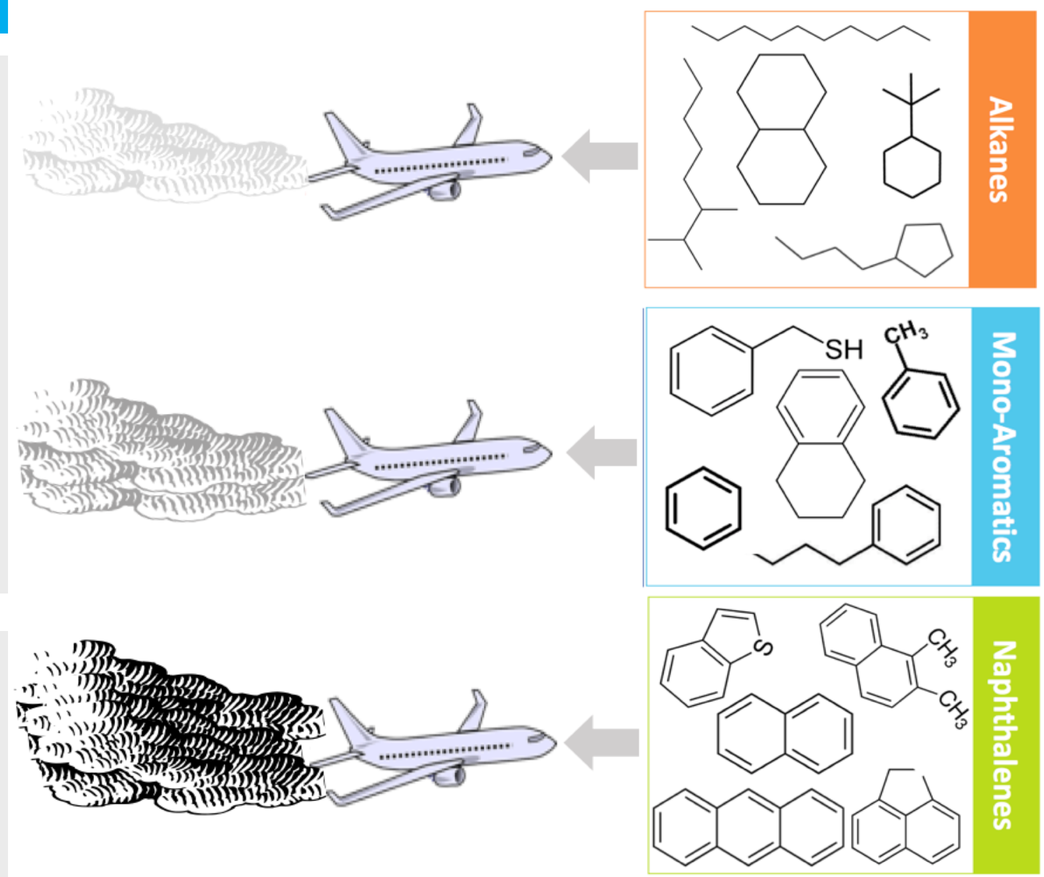
Motivation

nvPM cause and effect

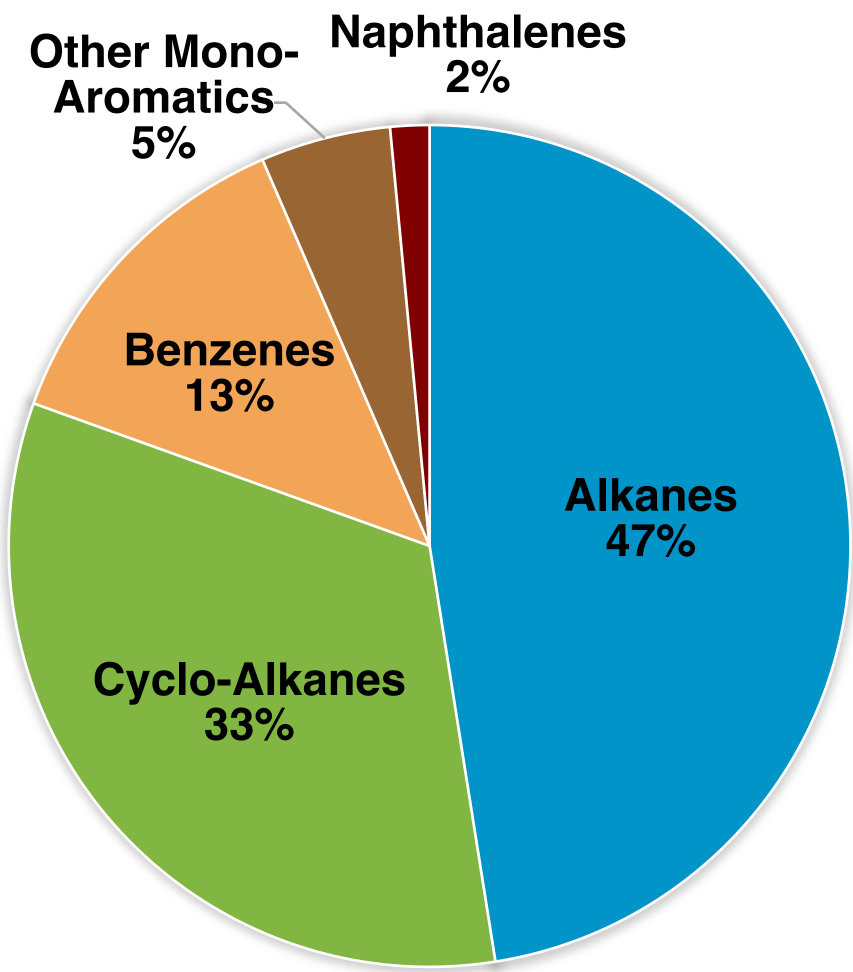
1 Aviation-attributable non-volatile particulate matter (nvPM) emissions contribute to:

- Air quality related **health effects** (Hoek et al. 2013)
- Aviation's climate impact through **direct & indirect radiative forcing** and **contrail formation**

2 Naphthalenes in jet fuel have been identified as **disproportionate contributors to nvPM emissions** compared to other fuel species (Moore et al. 2015, Brem et al. 2015)



Motivation



Typical jet fuel composition

Naphthalene Removal

3 On average, naphthalenes constitute **less than 2% of the total composition of jet fuel**, and less than 10% of the total aromatic content (PQIS, 2013)

4 There are **industry-standard finishing processes** that, with minimal changes, could be used to eliminate naphthalenes in jet fuel feedstocks (Gary et al. 2007)

Approach & Current Status

Project Goal

Conduct a U.S.-wide cost-benefit analysis of naphthalene removal

Research Steps

1. Develop **models of refinery processes** capable of removing naphthalene ✔
2. Calculate **investment and operating costs** associated with these processes ✔
3. Calculate **additional lifecycle GHG emissions** from refinery processing ✔
4. Estimate **reduction in nvPM emissions** from use of naphthalene-depleted fuel
5. Calculate **air quality impacts** of changes in emissions
6. Estimate **climate impacts** of changes in emissions

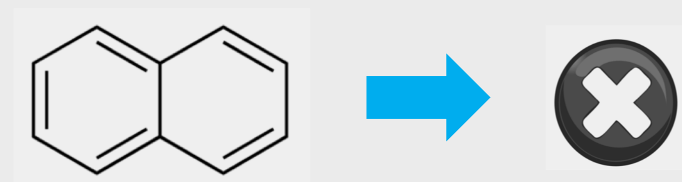
Refinery Processing Model

Hydro-Treating

- Industry standard finishing process
- Hydrogen and jet fuel reacted to:
  - **Saturate** di-aromatics
  - Remove **sulfur / nitrogen**

Extractive Distillation

- Di-aromatics selectively **removed** from jet fuel using a polar solvent
- Naphthalene component used or burned elsewhere in the refinery



Input Data
Refinery size & configuration, regional prices

→

Single Refinery Model
Capital & operating costs, emissions

→

Total Cost
NPV, price premium, cost breakdowns

Repeat for 116 U.S. refineries

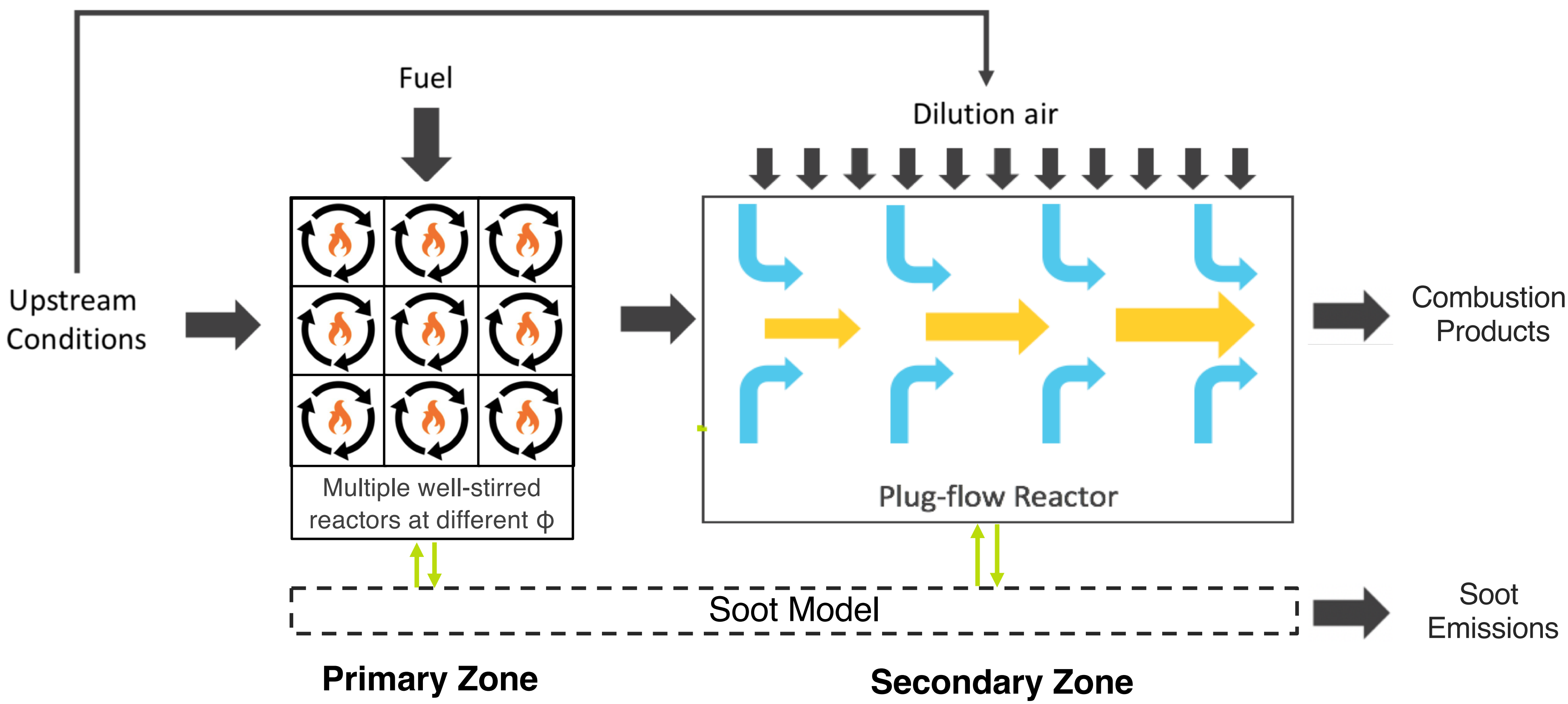
Monte Carlo simulation

nvPM Reduction: Literature Estimates

- **CFM-56 engine** studied using jet fuel seeded with varying levels of **naphthalene-rich or –depleted aromatic additive** (Brem et al. 2015). Observed nvPM reduction for 1.6 vol% naphthalene reduction:
  - 30% Engine Thrust: ~50% reduction
  - 65% Engine Thrust: ~30% reduction
  - 85% Engine Thrust: ~15% reduction
  - 100% Engine Thrust: ~0% reduction
- **T63 turboshaft engine** studied at "idle" and "cruise" conditions, using fuels with **varying aromatic and naphthalene contents** (Dewitt et al. 2008). Compare nvPM production from JP-8 and biofuel with 20% naphthalene-free aromatics. nvPM reductions were:
  - Engine Idle: 40% reduction
  - Engine Cruise: 15% reduction
- Estimated range of nvPM reductions from naphthalene-free fuel: 15-40%

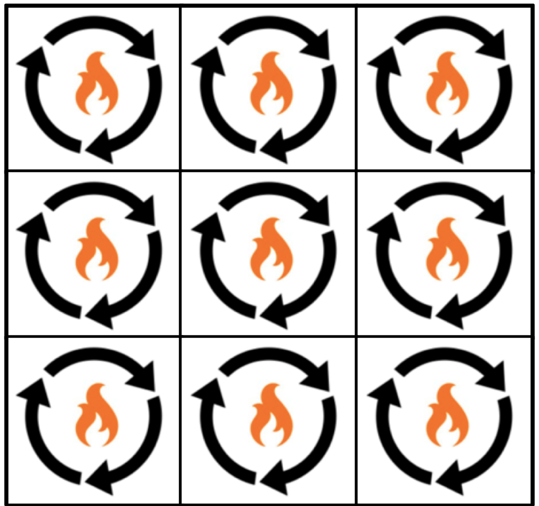
nvPM Reduction: Combustor Modeling

- Detailed-chemistry reactor network for nvPM estimation
  - **Reaction Mechanism Generator (RMG)** used to generate the jet-fuel combustion reaction mechanism
  - **Soot inception and microphysics** estimated through the combustor model
- Fuel composition study to estimate differential impact of **naphthalene and other fuel components** on soot production

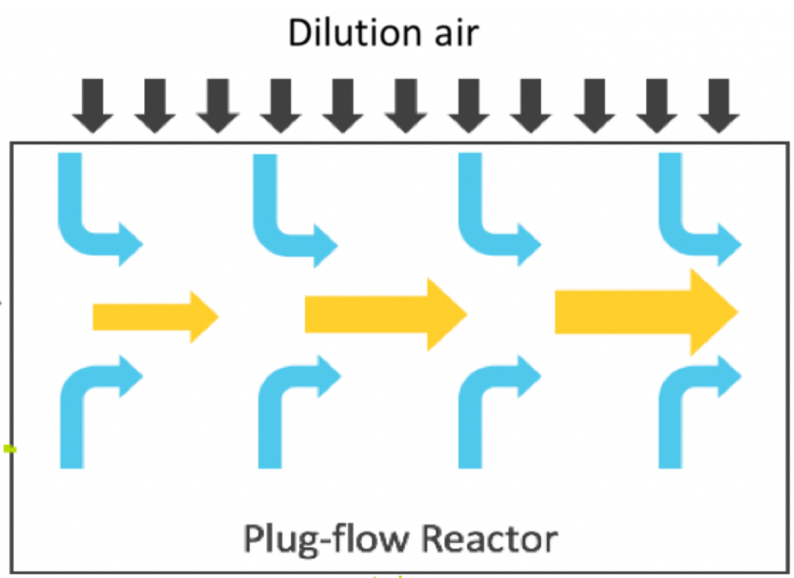


nvPM Reduction: Combustor Modeling

- Primary zone is fuel rich, so soot particles are expected to form here
- Multiple well-stirred reactors at different equivalence ratios are used in primary zone in order to account for mixture inhomogeneity in the primary zone
- Fuel composition influences PAH and soot formation rates



Multiple well-stirred reactors at different equivalence ratios

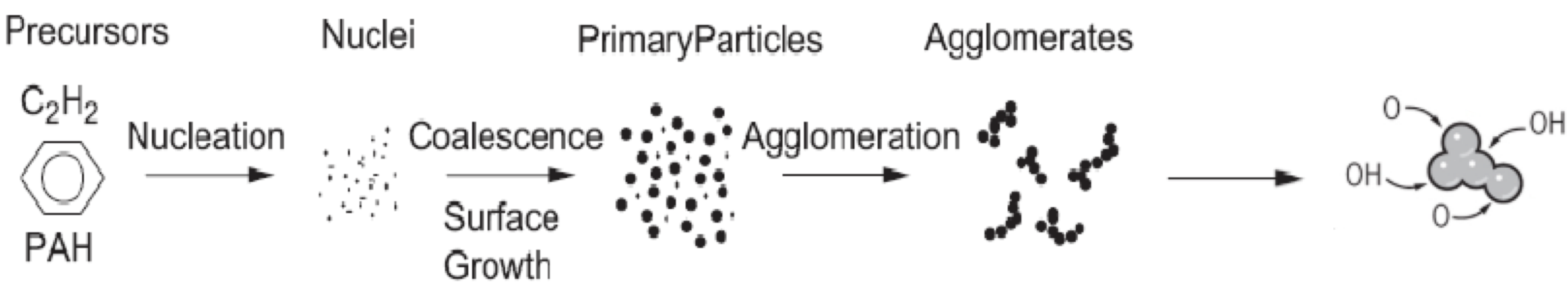


- Soot nucleation decreases as air is added in the secondary zone and equivalence ratio drops
- Dilution air oxidizes soot particles
- Modeled as a plug flow reactor with spatially-varying mixing of dilution and primary zone products

nvPM Reduction: Combustor Modeling

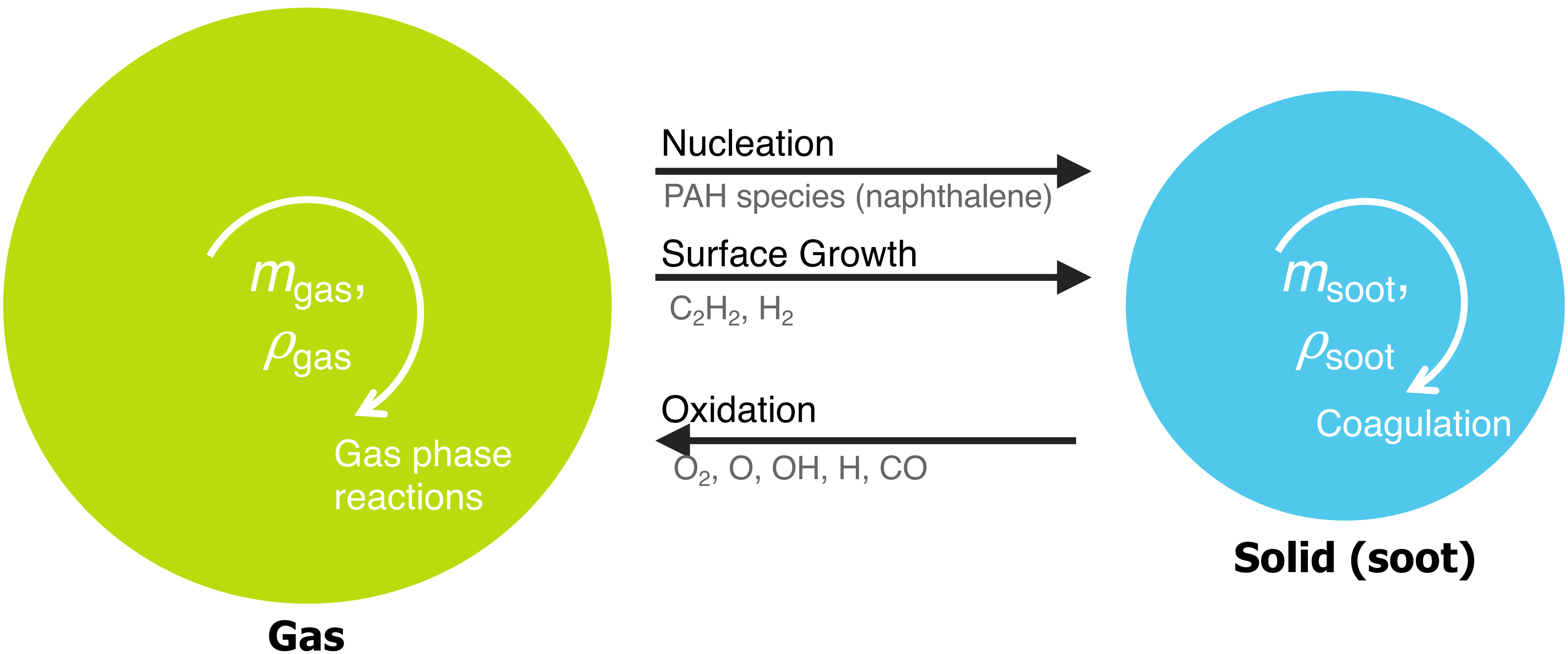
- Soot formation represented by four main steps
- Two-equation soot model implemented in combustor model to calculate both mass and number of soot particles

Nucleation → Surface Growth → Coagulation & Agglomeration → Oxidation



nvPM Reduction: Combustor Modeling

- Interactions between gas phase species and soot modeled through nucleation, surface growth and oxidation reactions
- Gas phase reactions and coagulation only affect composition of gas phase and size of soot particles respectively



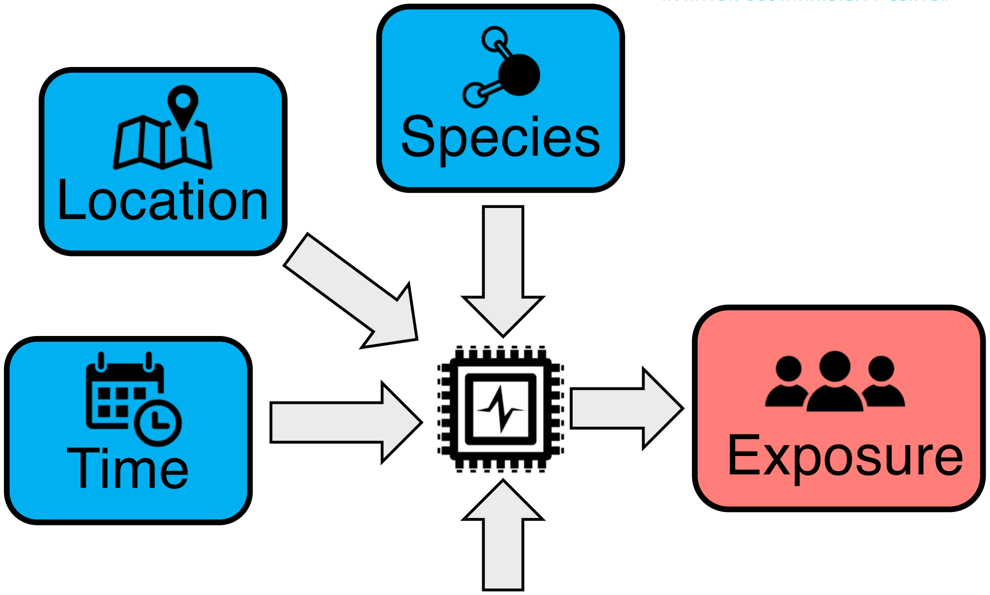
nvPM Environmental Impacts

Source	Air Quality Impact	Climate Impact	Description
Reduced nvPM	Reduced Mortalities	Cooling	Reduced soot emissions from aircraft engines
Contrail Effects	- - -	Mixed	Increased fuel hydrogen content Decreased particulate number
Refinery Emissions	- - -	Warming	Increased CO_2, light end emissions from hydrogen production / utilities
Reduced Sulfates*	Reduced Mortalities	Warming	Reduced fuel sulfur content

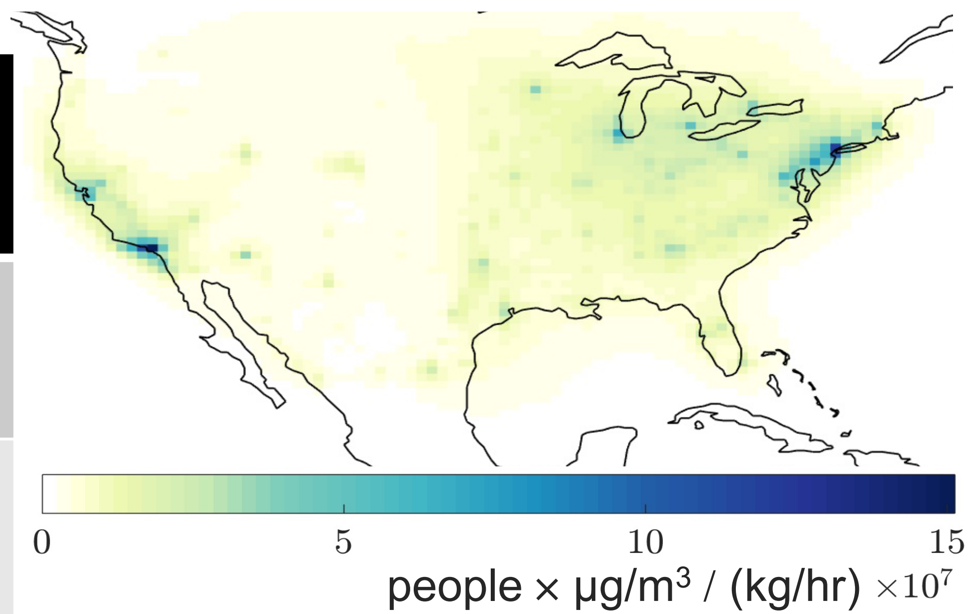
*Hydro-treatment will remove the majority of sulfates. Extractive distillation has limited impacts on sulfates.

Air Quality Impacts: Initial Estimates

- Consider nvPM emissions reduction of 15–40% and sulfur reduction of 97% (for HT)
- Use $PM_{2.5}$ sensitivities from GEOS-Chem regional adjoint model
- Evaluate monetized health impacts due to cardiovascular disease and lung cancer (Krewski et al. 2009)



sensitivities to nvPM emissions

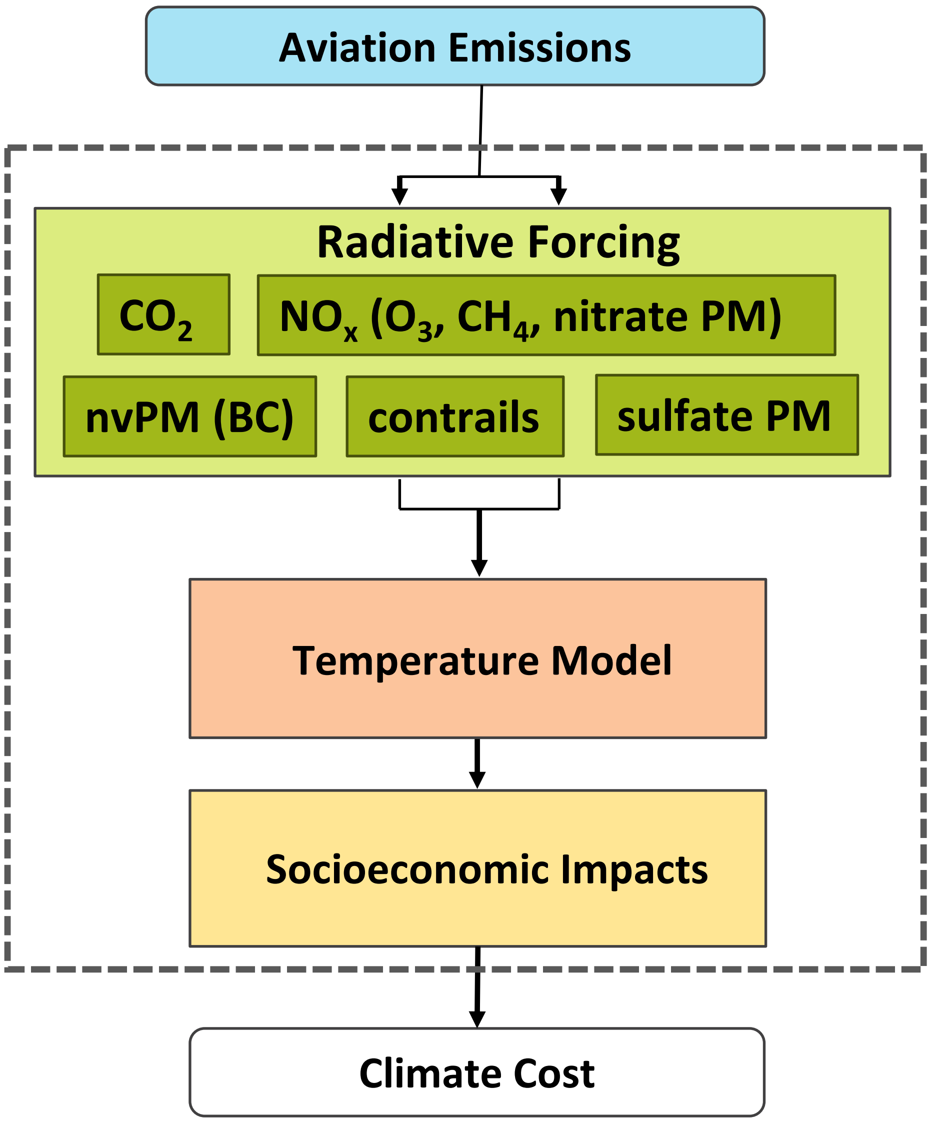


Impact Pathway	Monetized Benefits (¢/gallon)
nvPM	0.08 (0.02 – 0.16)
Sulfate PM	1.86 (1.05 – 2.67)

Climate: Preliminary Results

- Consider nvPM emissions reduction of 15–40% and sulfur reduction of 97% (for HT)
- Evaluate monetized climate costs using APMT-I Climate model
  - Suitable for evaluating RF changes for direct & indirect BC and sulfate PM
  - impact of changing nvPM emissions on contrails is considered separately

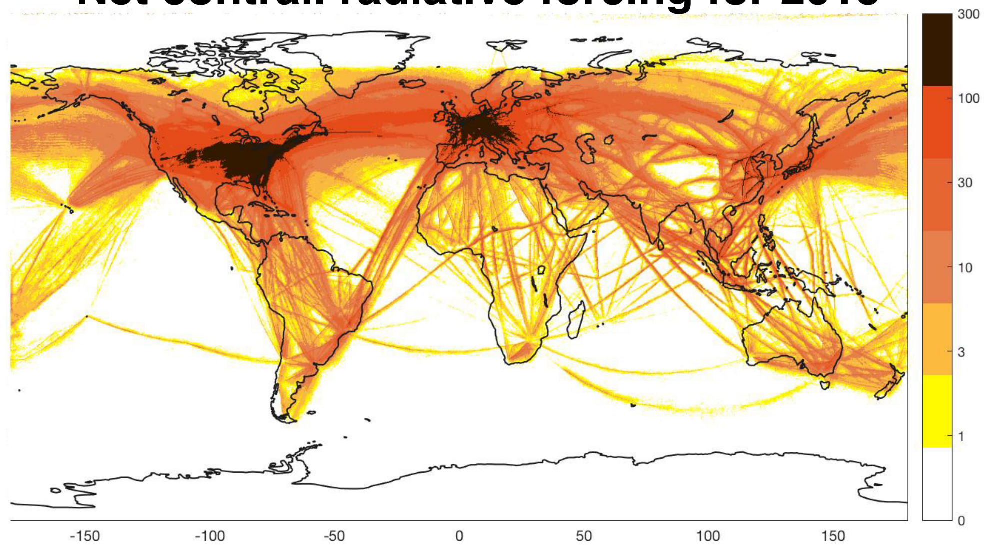
Impact Pathway	Cost (¢/gallon)
nvPM	-0.12 (-0.015 – -0.23)
sulfate*	4.14 (0.60 – 11.1)
Refinery CO_2	1.8 (0.31 – 5.12)



Effect of Fuel Properties on Contrails

- Contrails & contrail cirrus are estimated to be responsible for **~40% of aviation's net climate impact** (Grobler et al. 2019)
- Increase in water vapor emissions (higher fuel hydrogen content) causes contrails to **form more frequently**

Net contrail radiative forcing for 2015



- Decrease in number of ice crystals results in **larger ice crystals**, which fall faster, making contrails **shorter-lived**
- Contrails composed of fewer ice crystals have **lower optical depth**
- Complex effect on net radiative forcing due to competing warming & cooling effects

Evaluating Contrail Impacts

- Total contrail impacts have a monetized value of 25 ¢/gallon (3 – 69) (Grobler et al. 2019)
- **First-order impact estimate:** Use contrail simulations of the effect of ice nuclei (IN) emissions reductions on radiative forcing (RF):
  - Caiazzo et al. (2017) found reducing IN by 67% reduced contrail RF by <13%
  - Burkhardt et al. (2018) found that reducing IN by 50% reduced contrail RF by ~20%
  - For nvPM reductions of 15 – 40%, estimate reduction in contrail RF of 7% (4 – 13%), or 1.7 ¢/gallon (0.4 – 5.3)
- **Ongoing work:**
  - Use a Lagrangian contrail model to simulate effect of changing fuel composition on contrail properties on a flight-by-flight basis
  - Include effect of sulfur removal on availability of IN

Preliminary U.S.-Wide Cost-Benefit Analysis

	Component	Hydrotreatment (¢/gallon)		Extractive Distillation (¢/gallon)	
Processing	Refinery	9.1	(7.6 – 10.2)	6.4	(5.7 – 7.6)
Air quality	nvPM	-0.1	(-0.02 – -0.16)	-0.1	(-0.02 – -0.16)
	Sulfur	-1.9	(-1.0 – -2.7)	0	
Climate	nvPM	-0.2	(-0.02 – -0.6)	-0.2	(-0.02 – -0.6)
	Sulfur	3.9	(0.6 – 10.5)	0	
	Contrails	-1.7	(-0.4 – -5.3)	-1.7	(-0.4 – -5.3)
	Refinery	1.8	(0.3 – 4.5)	1.8	(0.3 – 4.8)
Net unit cost (¢/gallon)		**10.9**	**(5.8 – 16.8)**	**6.3**	**(2.4 – 9.3)**
Net U.S. cost (billion USD/year)		**1.5**	**(0.8 – 2.3)**	**0.9**	**(0.3 – 1.3)**

Median values and 95% CIs shown for each component.

Positive values indicate net costs.

Conclusions

- Removing naphthalenes from jet fuel could reduce nvPM emissions by 15-40%
- There are viable refinery processes for removing naphthalenes from jet fuel
- Climate benefits of naphthalene removal are largely offset by additional CO_2 emissions at the refinery
- System-wide removal of naphthalene is unlikely to be cost beneficial
- Lack of benefit for the simplest policy option suggests consideration of selective naphthalene removal
- Evaluating situations where selective removal provides benefits requires further refinement of AQ and contrail impact estimates

Future Work

- Continue improving AQ and climate (contrail) impact estimates
- Develop scenarios for selective naphthalene removal, e.g. airport-specific or flight-specific use of naphthalene-free fuel and conduct cost benefit analyses
- Use combustor model to identify fuel components which reduce soot emissions while still meeting jet fuel specifications
- Apply methods for determining AQ and climate impacts to evaluate benefits of (sulfur-free, paraffinic / naphthalene-free) biofuels

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