FAA CENTER OF EXCELLENCE FOR ALTERNATIVE JET FUELS & ENVIRONMENT

Naphthalene Removal Assessment

Project 39

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ASCENT
AVIATION SUSTAINABILITY CENTER

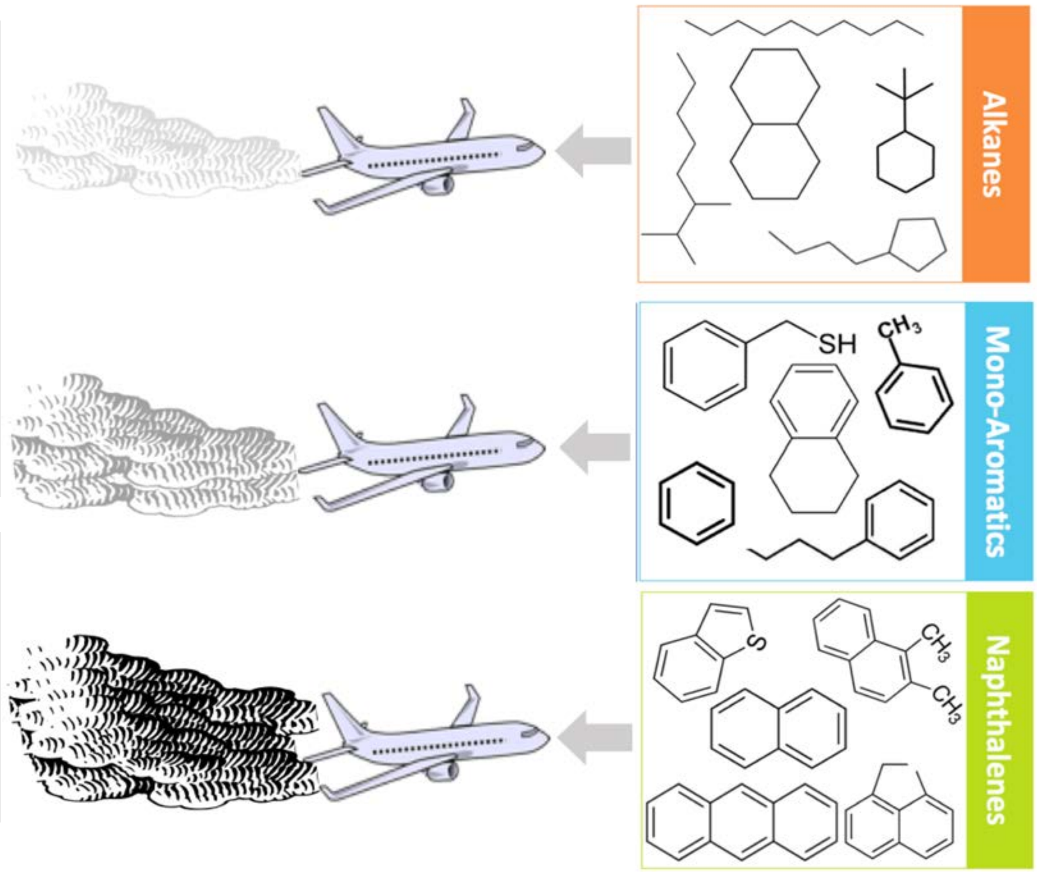
Motivation

NvPM cause and effect

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

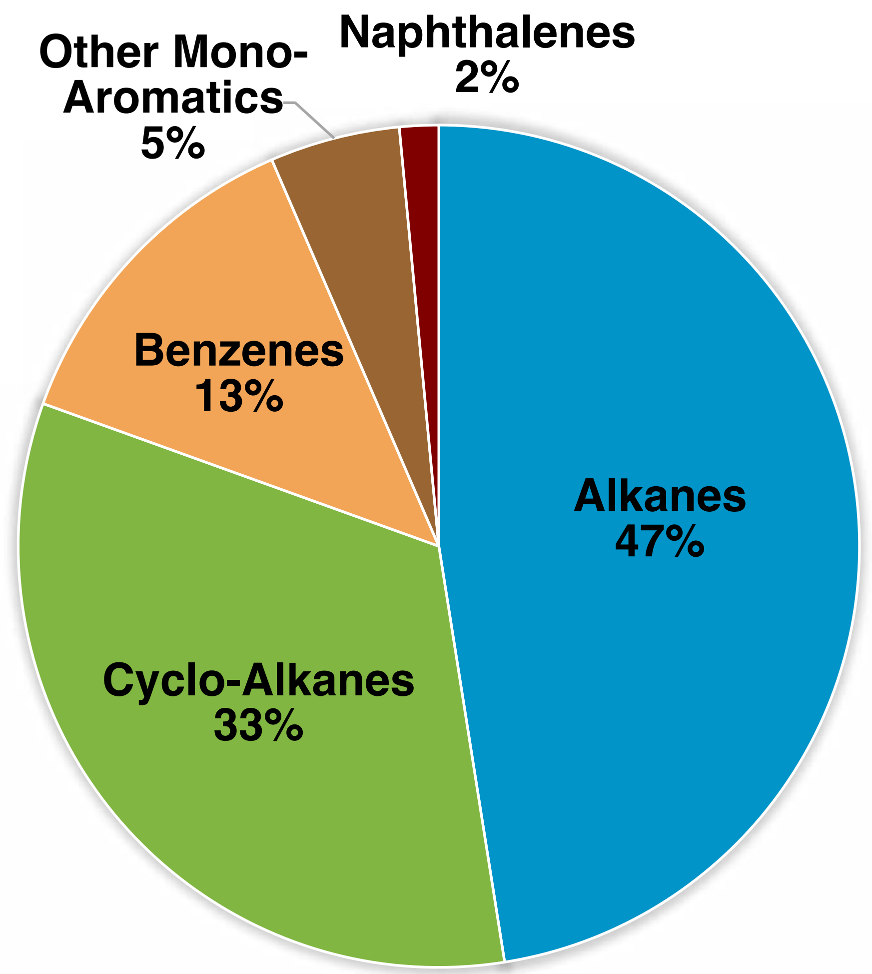
- Air quality related **health effects**
- Aviation's climate impact through **direct & indirect radiative forcing** and **contrail formation**

2 Naphthalenes in jet fuel have been identified as **disproportionate contributors to nvPM emissions** compared to other fuel species



G. Hoek *et al.*, *Environmental Health*, vol. 12, p. 43, 2013.
R. H. Moore *et al.*, *Energy Fuels*, vol. 29, no. 4, pp. 2591–2600, Apr. 2015.
B. T. Brem *et al.*, *Environ. Sci. Technol.*, vol. 49, no. 22, pp. 13149–13157, Nov. 2015.

Motivation



Typical jet fuel composition

Naphthalene Removal

4 On average, naphthalenes constitute **less than 2% of the total composition of jet fuel**, and less than 10% of the total aromatic content

3 There are **industry-standard finishing processes** that, with minimal changes, could be used to eliminate naphthalenes in jet fuel feedstocks

J. H. Gary, G. E. Handwerk, and M. J. Kaiser, CRC Press, 2007.
"Petroleum Quality Information System 2013 Annual Report," Jan. 2013.

Approach & Current Status

Project Goal

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

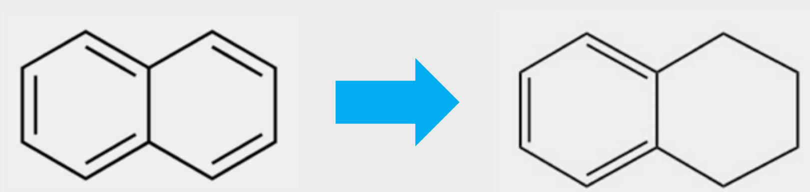
Research Steps

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

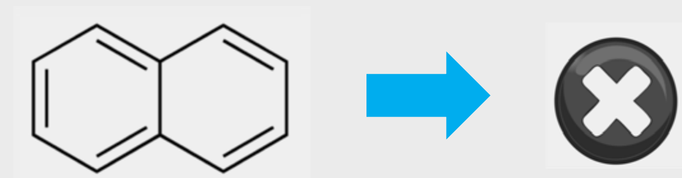
Hydro-Treating

- 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 raffinate used or burned elsewhere in the refinery



Input Data
Refinery size & configuration, regional prices

→

Single Refinery Model
Capital & operating costs, emissions

→

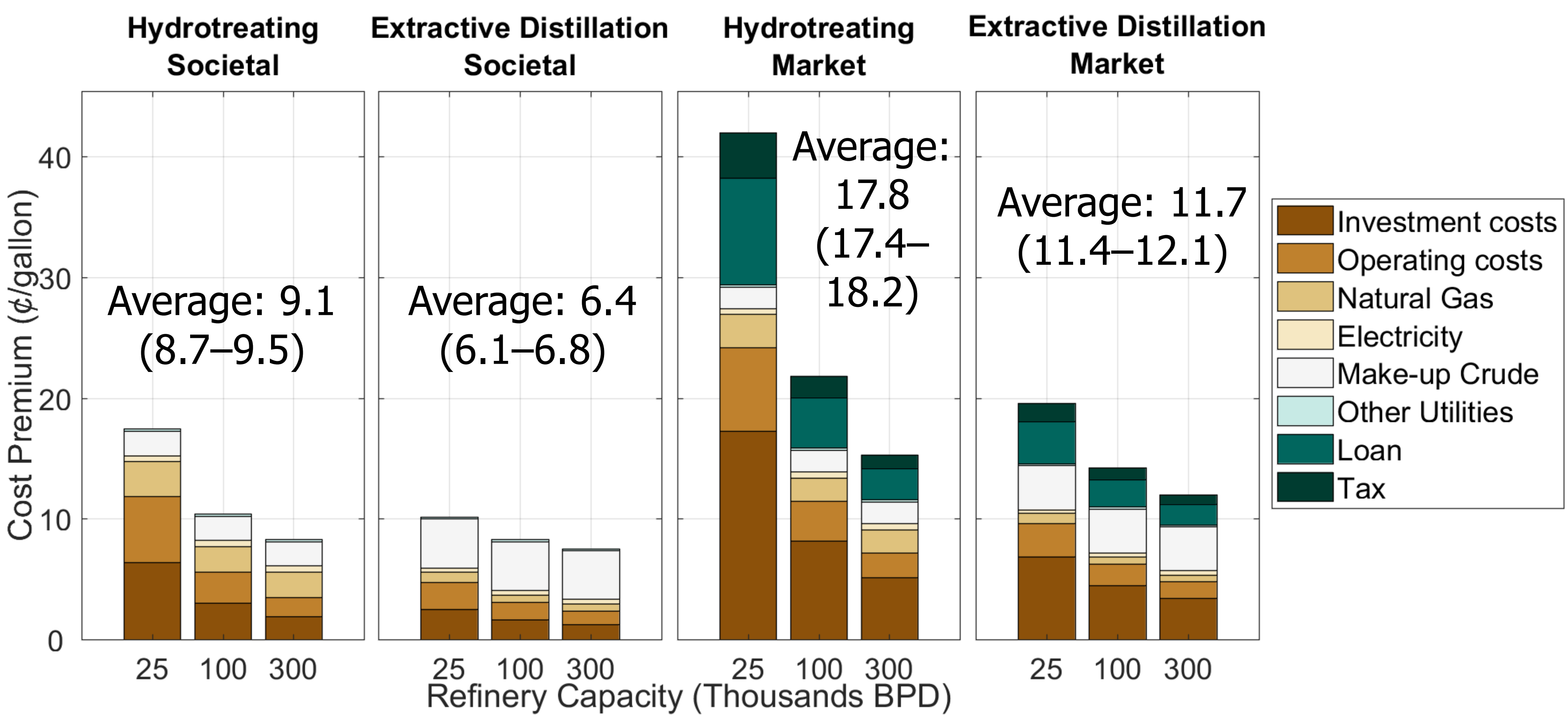
Total Cost
NPV, price premium, cost breakdowns

Repeat for 116 U.S. refineries

Monte Carlo simulation

Refinery Processing Costs

- **Market perspective**: Used to estimate the **impact of jet fuel market price**, based on the expected return of refiners
- **Societal perspective**: Used for **comparison to the benefits** of climate and air quality, which impact society as a whole

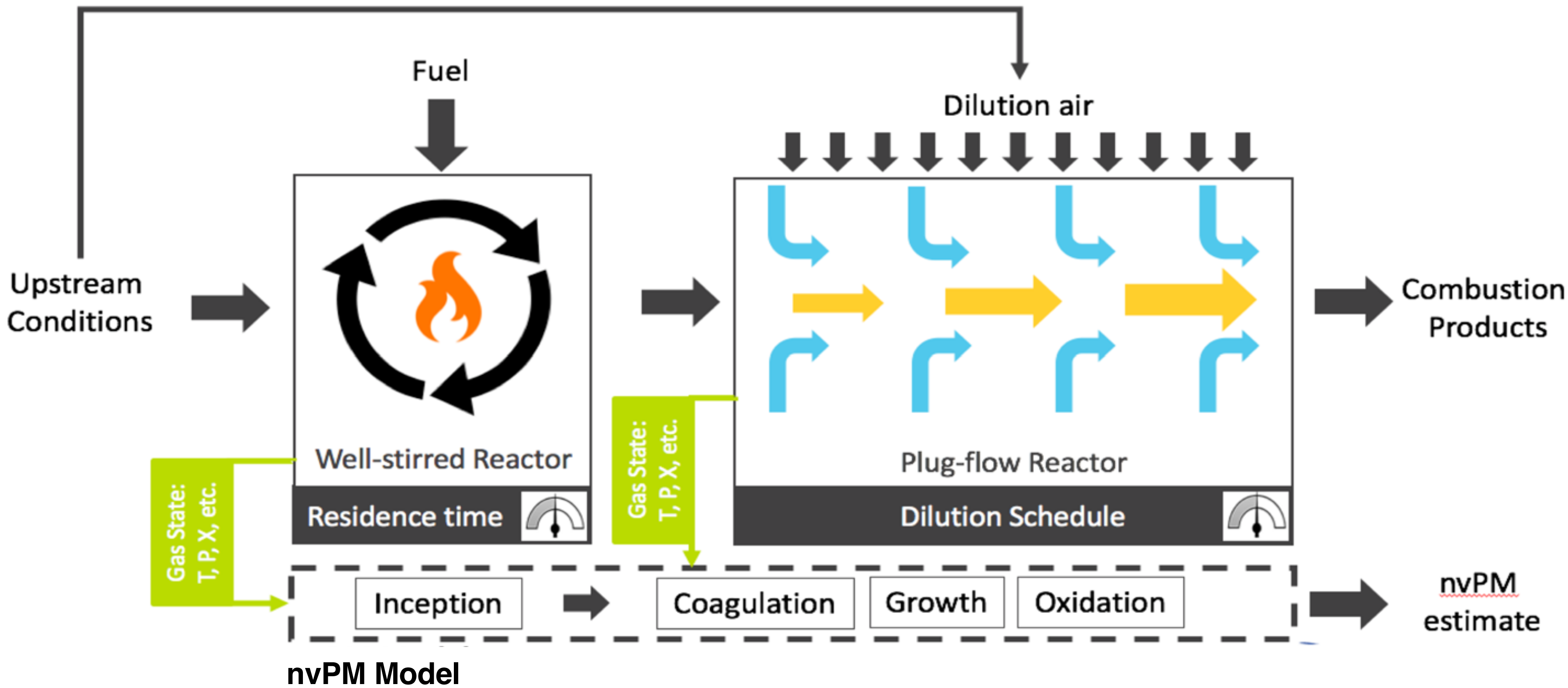


nvPM Reduction: Literature Estimates

- **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
- Assumed 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 **naphthalene's differential impact** on soot production



nvPM Environmental Impacts

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

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

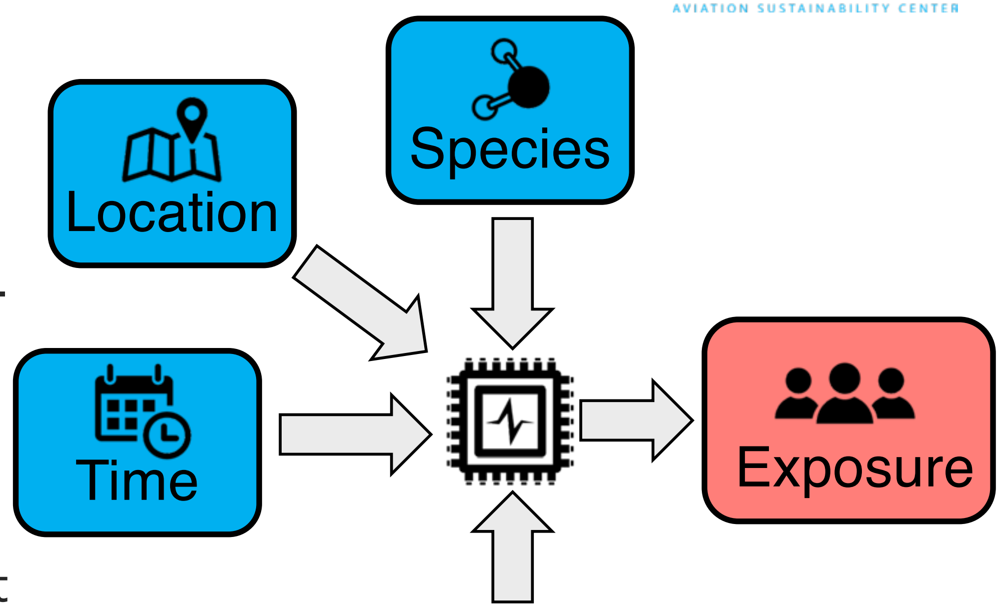
Refinery Processing Emissions

- Utilities used in the refinery generate CO_2 emissions
  - Natural gas used for process heat and H_2 production
  - Electricity
  - Light ends used for process heat
  - Byproduct naphthalene used for process heat
  - Upstream crude emissions for make-up jet fuel

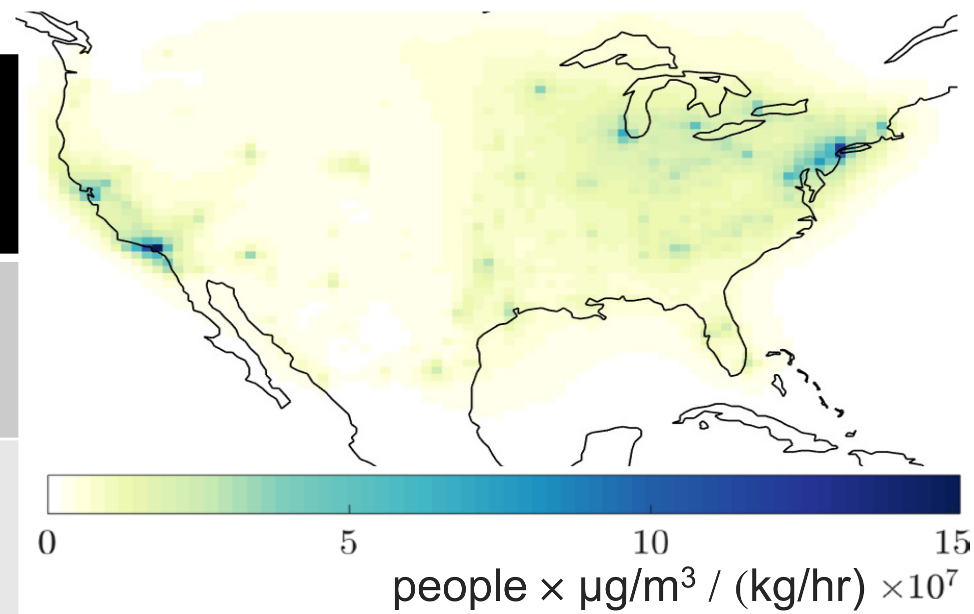
Parameter	Hydro-Treating	Extractive Distillation
Incremental EI	**3.35 gCO_2 / MJ**	**3.12 gCO_2 / MJ**
Increase in Well-to-Pump EI	17.5%	16.3%
Increase in Well-to-Wake EI	3.7%	3.4%

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

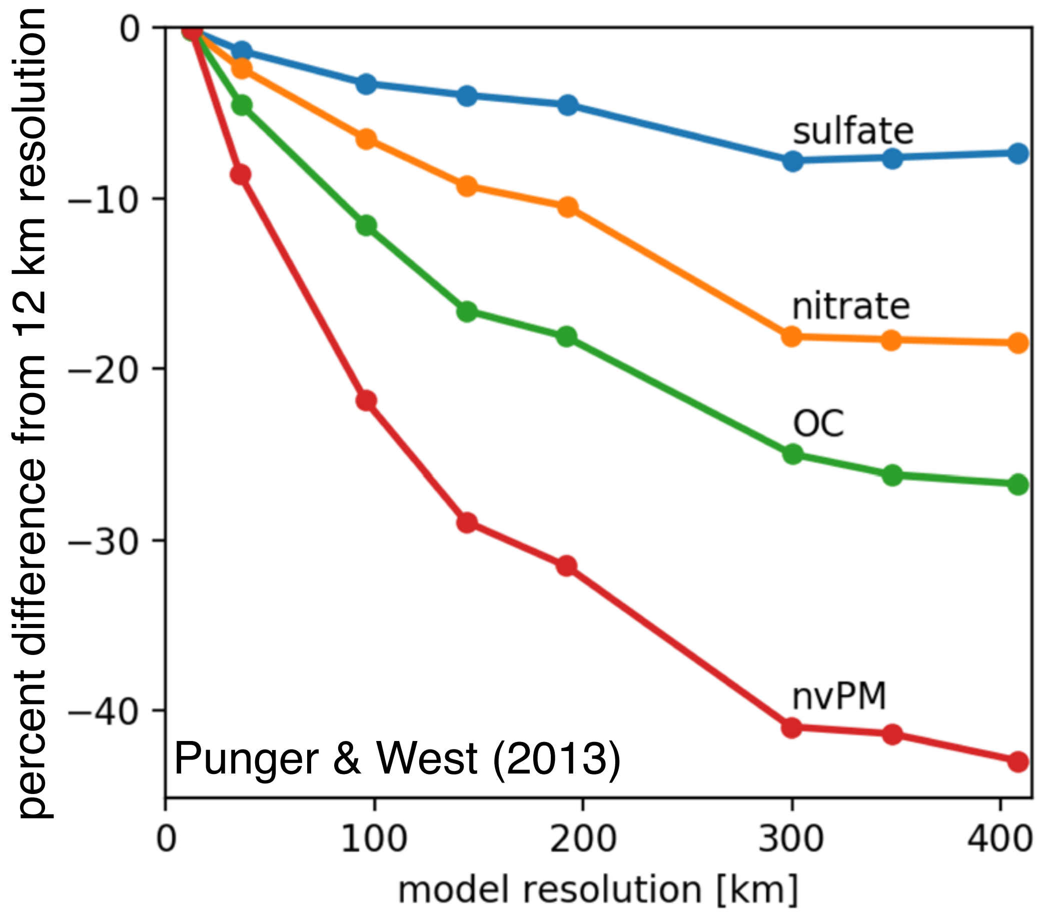


Impact Pathway	Monetized Benefits (¢/gallon)
nvPM	0.08 (0.02 – 0.16)
Sulfate PM	1.86 (1.05 – 2.67)

Air Quality Model Resolution

Challenge

- Air quality impact estimates depend on model resolution
- Low resolution models underpredict impacts
- Discrepancies are species-dependent
- Largest discrepancies are for nvPM



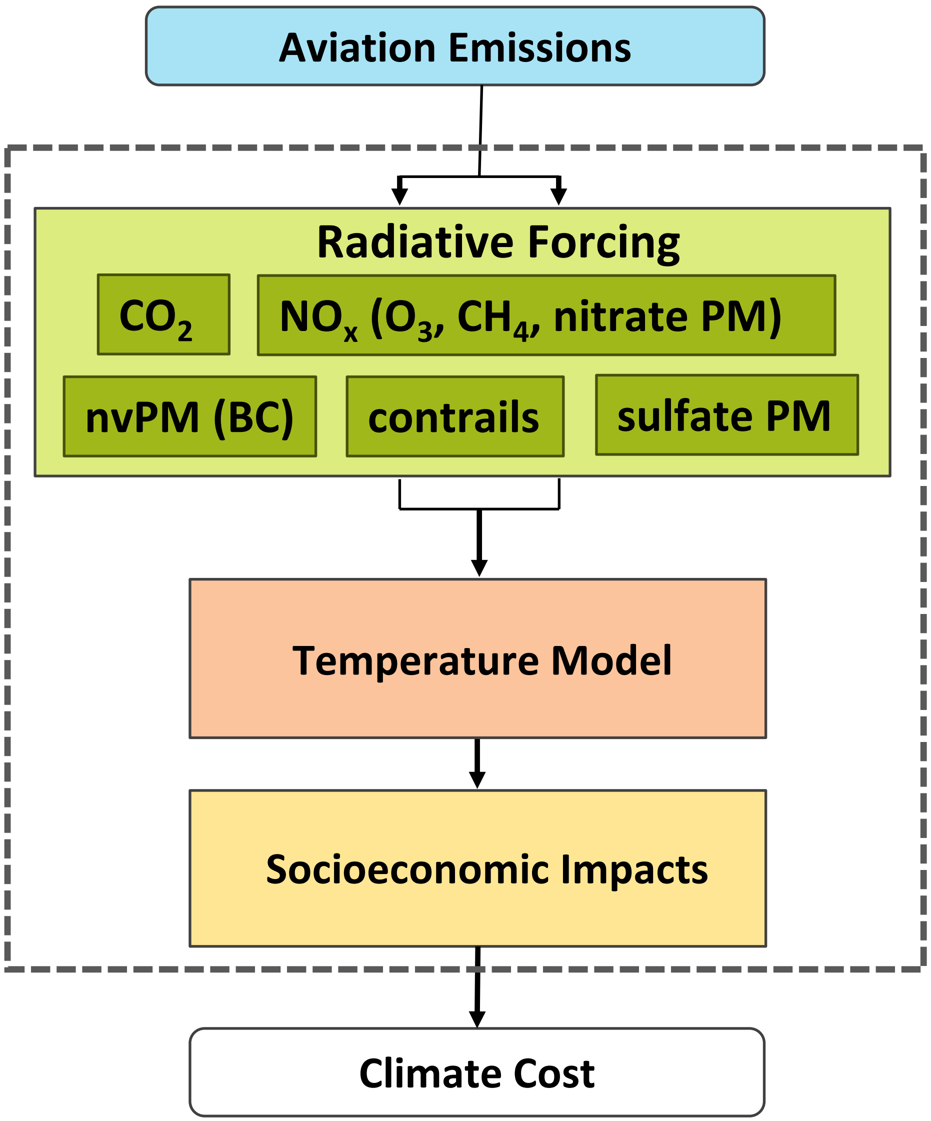
Approach

- Run higher-resolution regional AQ models without chemistry
- Apply existing reduced order, high-resolution and downscaling approaches (Wang et al 2014; Tessum et al, 2017)

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
  - Does not currently include impact of changing nvPM emissions on contrails

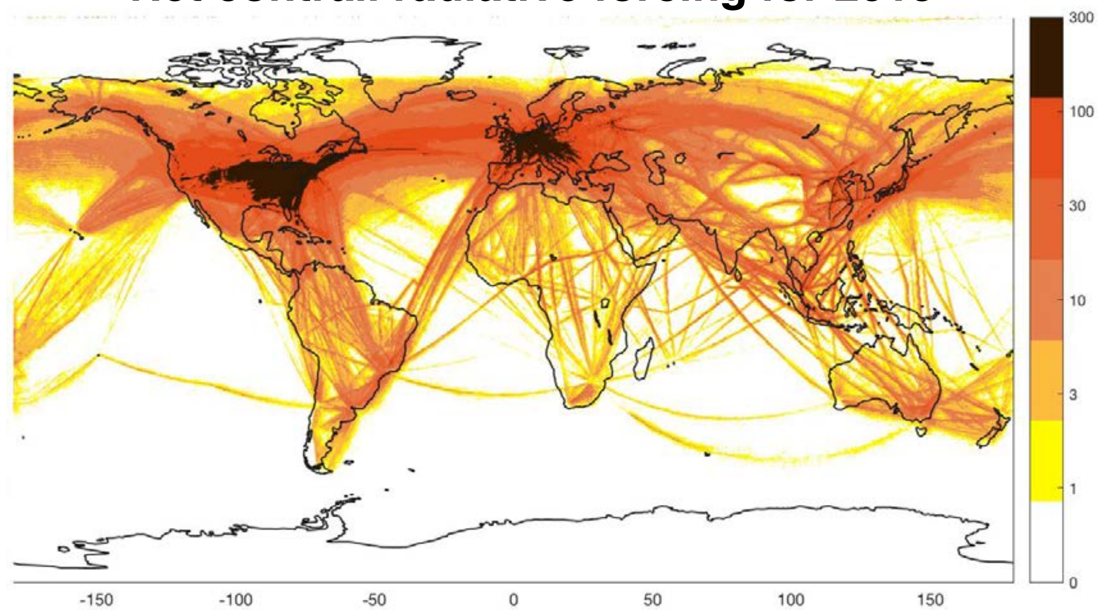
Impact Pathway	Cost (¢/gallon)
nvPM	-0.12 (-0.015 – -0.23)
sulfate*	4.14 (0.60 – 11.1)
Refinery CO_2	1.90 (0.31 – 5.12)



Climate Impacts: Contrail Model

- Contrails & contrail cirrus are estimated to be responsible for **~40% of aviation's net climate impact** on a NPV basis
- Use the Contrail Evolution and Radiation Model (CERM) to evaluate the role of **fuel properties** on contrail radiative forcing
  - Flight tracks & meteorological data used to evaluate contrail formation
  - Track persistent contrails and model growth, settling, diffusion, and evaporation
  - Calculate shortwave and longwave radiative forcing based on ice crystal properties

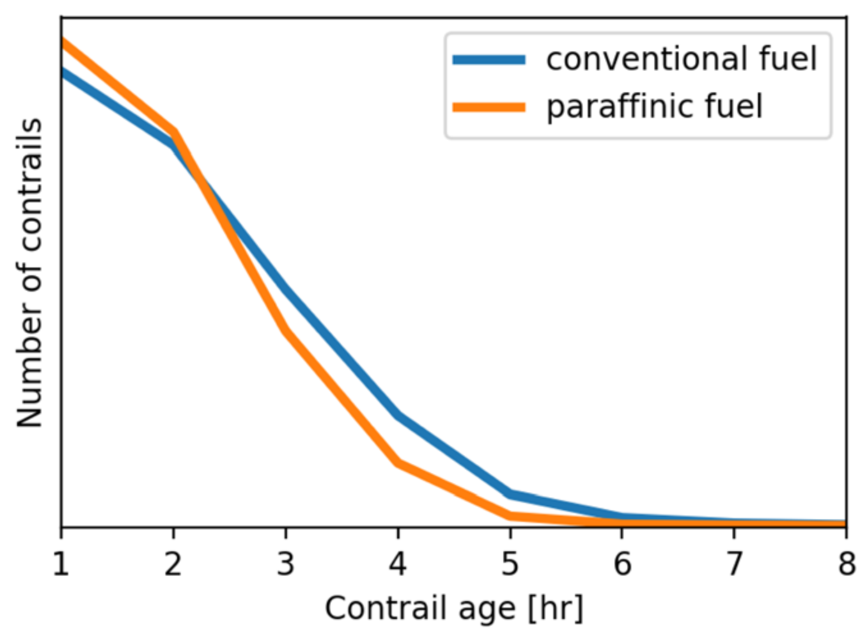
Net contrail radiative forcing for 2015



Effect of fuel properties on contrails

- Used CERM to simulate effect of paraffinic biofuels on contrail properties for US-origin flights
- Change in water emissions & heating value causes contrails to **form more frequently**
- 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

	Conventional Fuel	Paraffinic Fuel
EI(ice nuclei) [10^{15}/kg_{fuel}]	1.0	0.31
EI(H_2O) [kg/kg_{fuel}]	1.23	1.37
LHV [MJ/kg]	43.1	44.1



Partial Cost-Benefit Analysis

	Component	Hydrotreatment (¢/gallon)		Extractive Distillation (¢/gallon)	
Air quality	nvPM	-0.1	(-0.02 – -0.16)	-0.1	(-0.02 – -0.16)
	Sulfur	-1.9	(-1.1 – -2.7)	0	
Climate	nvPM	-0.2	(-0.02 – -0.6)	-0.2	(-0.02 – -0.6)
	Sulfur	4.1	(0.6 – 11.1)	0	
	Contrails	*unknown*		*unknown*	
	Refinery	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)**

Median values and 95% CIs shown for each component.
Positive values indicate net costs.

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