Naphthalene Removal Assessment

Project 39

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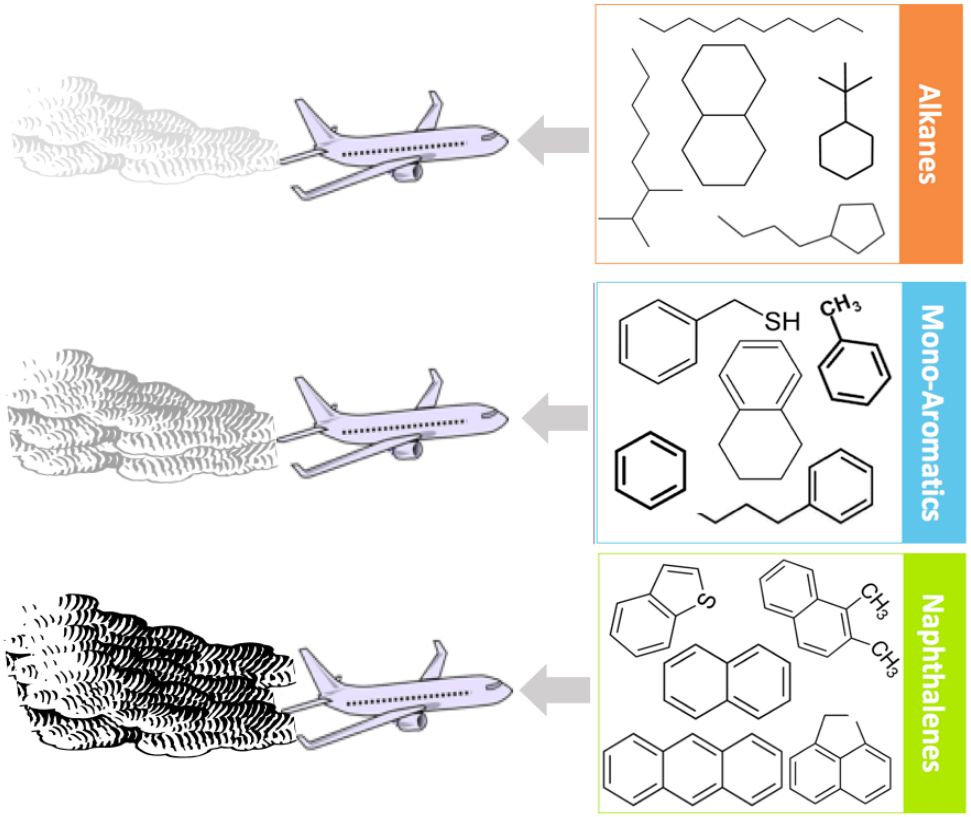
AVIATION SUSTAINABILITY CENTER

Motivation

NvPM cause and effect

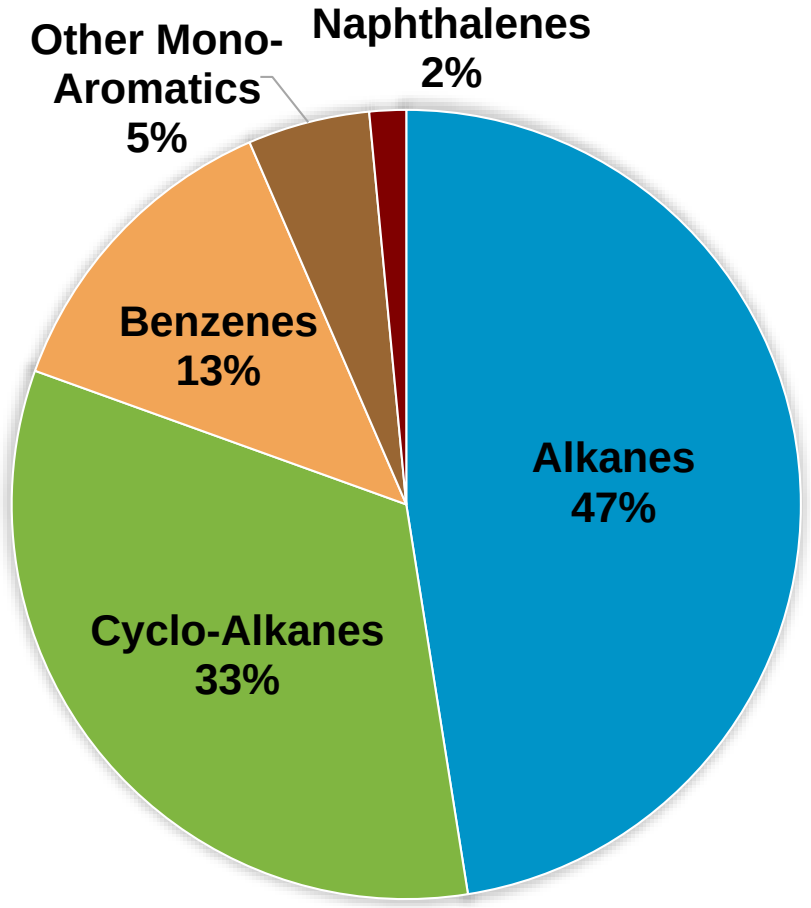
1. Aviation-attributable non-volatile particulate matter (nvPM) emissions contribute to:
   - Air quality related **health effects**
   - Aviation's climate impact through **direct & indirect radiative forcing** and **contrail formation**

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 that 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.

Motivation

NvPM cause and effect

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- Air quality rela…
- Aviation's clim… direct **radiative… contrail formati…**

2 Naphthalenes in jet fuel have been identified as a **disproportionate contributor to nvPM emissions** when compared to mono-aromatic species

Naphthalene Removal

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3 On average, **naphthalenes constitutes less that 2%** of total composition of jet fuel, and less that 10% of total aromatic content

A U.S.-wide cost-benefit analysis of naphthalene removal is desirable to inform future Jet-A standard policy

Current work and status

1 Completed

1a Select **candidate refinery processes** for naphthalene removal ✓

1b **Calculate investment and operating costs** for selected processes ✓

1c Estimate **the cost of removing naphthalene** from the U.S. jet pool ✓

Estimate **added refinery emissions** associated with additional jet fuel processing ✓

2 Near Term Objectives

2a **Estimate reduction in nvPM** due to reduced fuel naphthalene content (✓)

2b Quantify **climate and air quality impacts**

2c Complete integrated **U.S. societal cost/benefit analysis** of nvPM reduction

1a Completed: Candidate refinery processes

Objectives

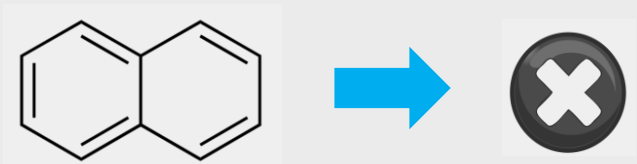
- Select candidate refinery processes that selectively remove jet fuel naphthalenes while providing:
  - Preserved **aromatic content**; Minimal changes to fuel characteristics
  - **Limited incremental emissions**; Technical and economic **feasibility**

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



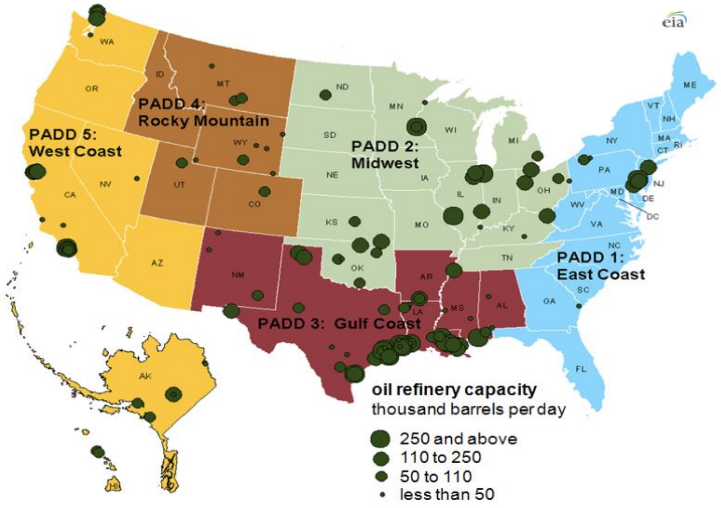
1b Completed: Calculated refinery process costs (1/2)

Objectives

- Determine **U.S. refinery pool capacity requirements** and:
  - Associated **utility and materials requirements** for each refinery
  - Process unit **investment and integration costs** and uncertainty
  - **U.S. regional utility costs**, cost growth, and uncertainty

U.S. Refining Pool Capacity

- 1.6 Million barrels/day jet fuel refining capacity
- 116 U.S. refineries considered
  - Capacities >1000 barrels per day of crude

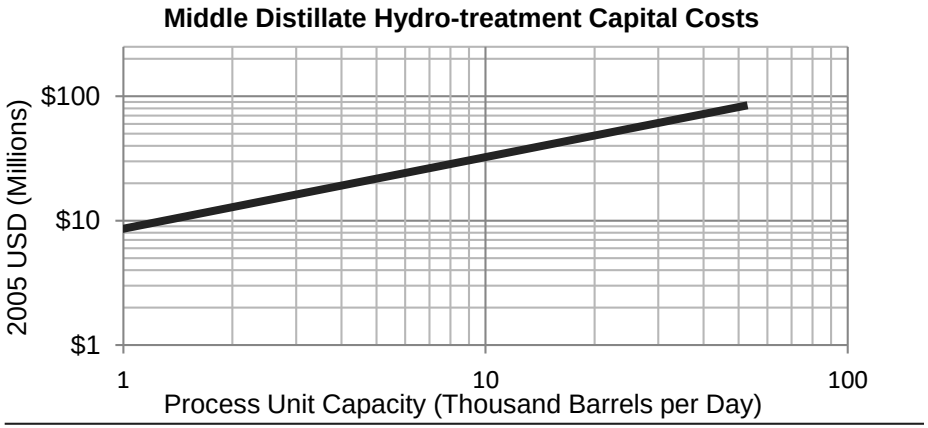


"Annual Energy Outlook 2017: with projections to 2050," U.S. Energy Information Administration, Jan. 2017.
"GlobalData O&G," *O&G: Downstream Analytics*. April 2017

1b Completed: Calculated refinery process costs (2/2)

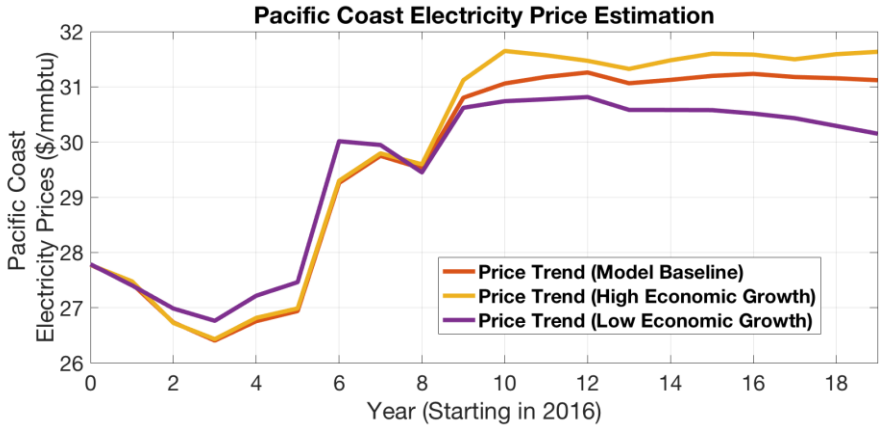
Capital Investment Costs

- Process unit and supporting units investment costs determined using cost-curve methods
- Other costs considered:
  - Utility system infrastructure
  - Integration costs
  - Inflation & **Location factors**



Operating Costs

- **U.S regional utilities historical and predictive data** collected
- Future utilities costs predicted as a function of
  - U.S. EIA **predicted mean**
  - **Stochastic term** calibrated by historical price fluctuations



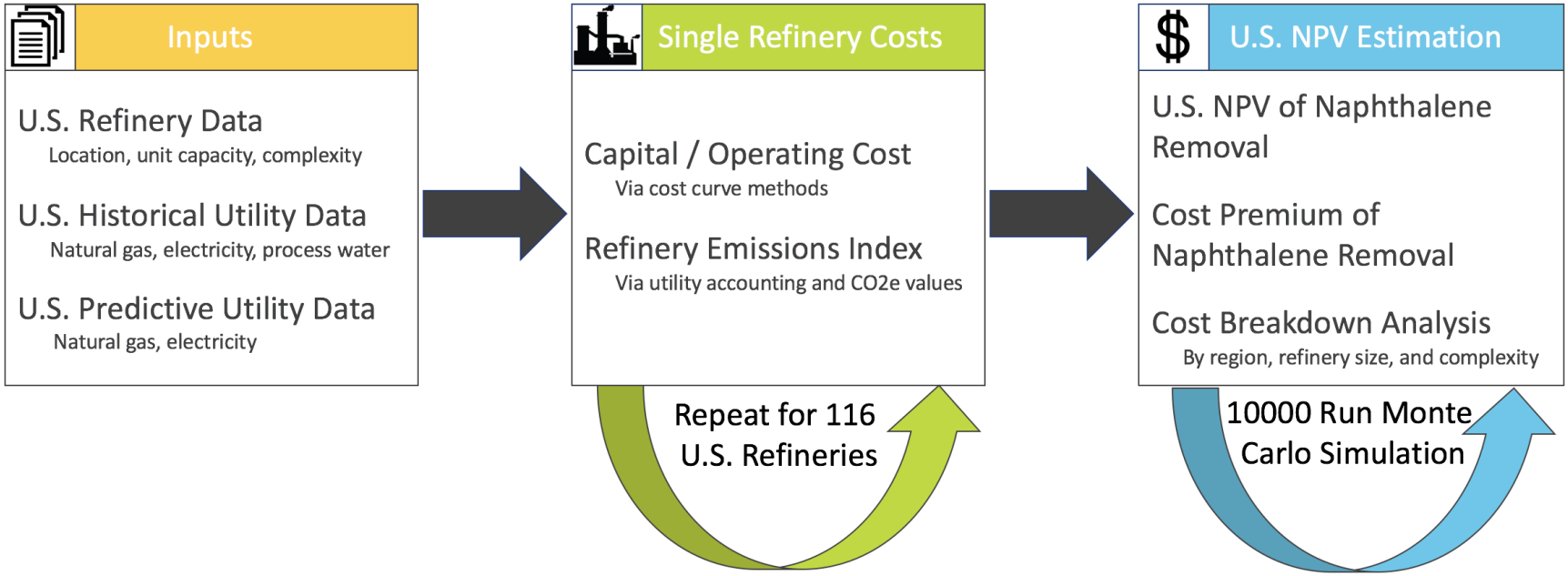
Uncertainties in cost accounted for as **parameter probability distributions**

J. H. Gary, G. E. Handwerk, and M. J. Kaiser, *Petroleum Refining: Technology and Economics, Fifth Edition*. CRC Press, 2007.

1c Completed: The costs naphthalene removal (1/2)

Objectives

- Collect capital and utility costs for U.S. refining pool
- Estimate the **integrated costs of naphthalene removal**
  - **Societal, integrated cost estimate** for U.S. produced jet fuel
  - Quantify uncertainty distributions due to uncertainties in model inputs

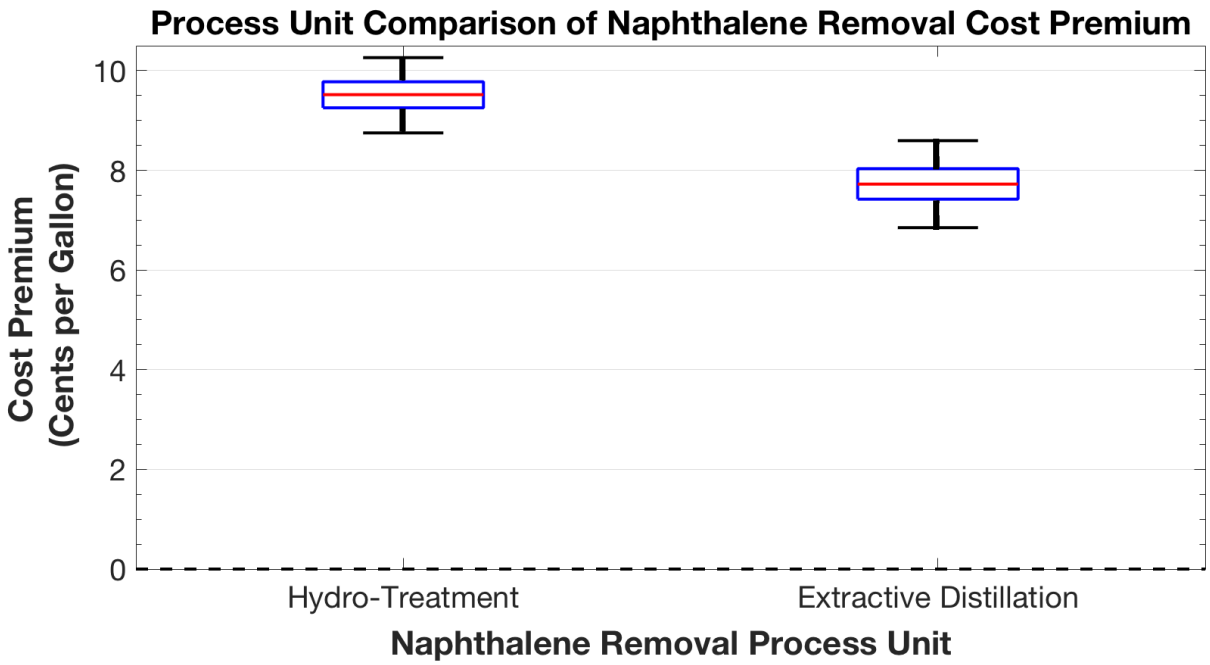


1c Completed: The costs naphthalene removal (2/2)

Hydro-treatment
9.51¢/gal (8.73, 10.26)*

Extractive Distillation
7.73 ¢/gal (6.81, 8.60)*

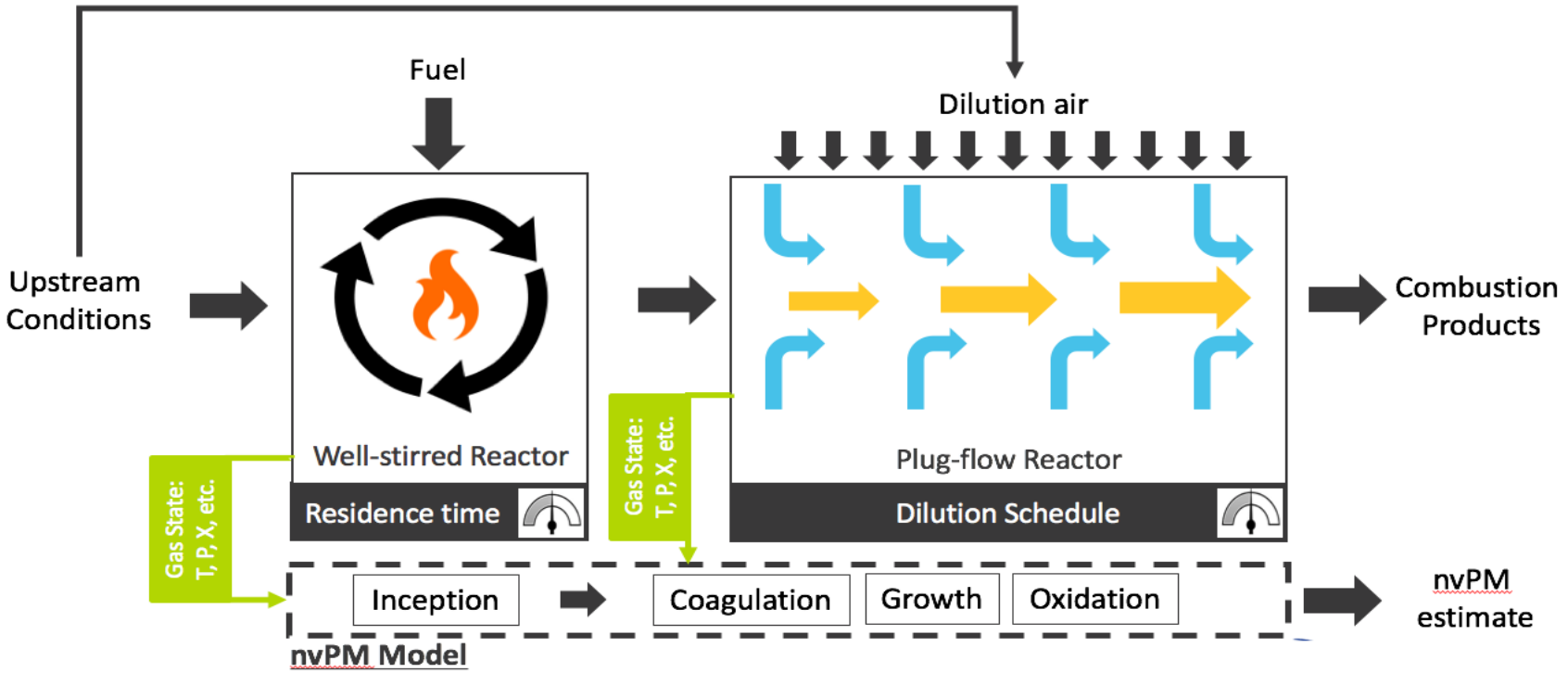
* 95% Confidence Intervals



- **U.S. societal cost estimate** (shown above) assumes funding structure is equivalent to U.S. federal bonds
- **Open-market cost premium will be higher** due to expected return on investment for investors, taxation, and loan guarantees. Mean cost premiums:
  - Hydro-Treating: 18 ¢/gal
  - Extractive distillation: 13 ¢/gal

2a Near term objectives: Link between naphthalene and nvPM

- 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



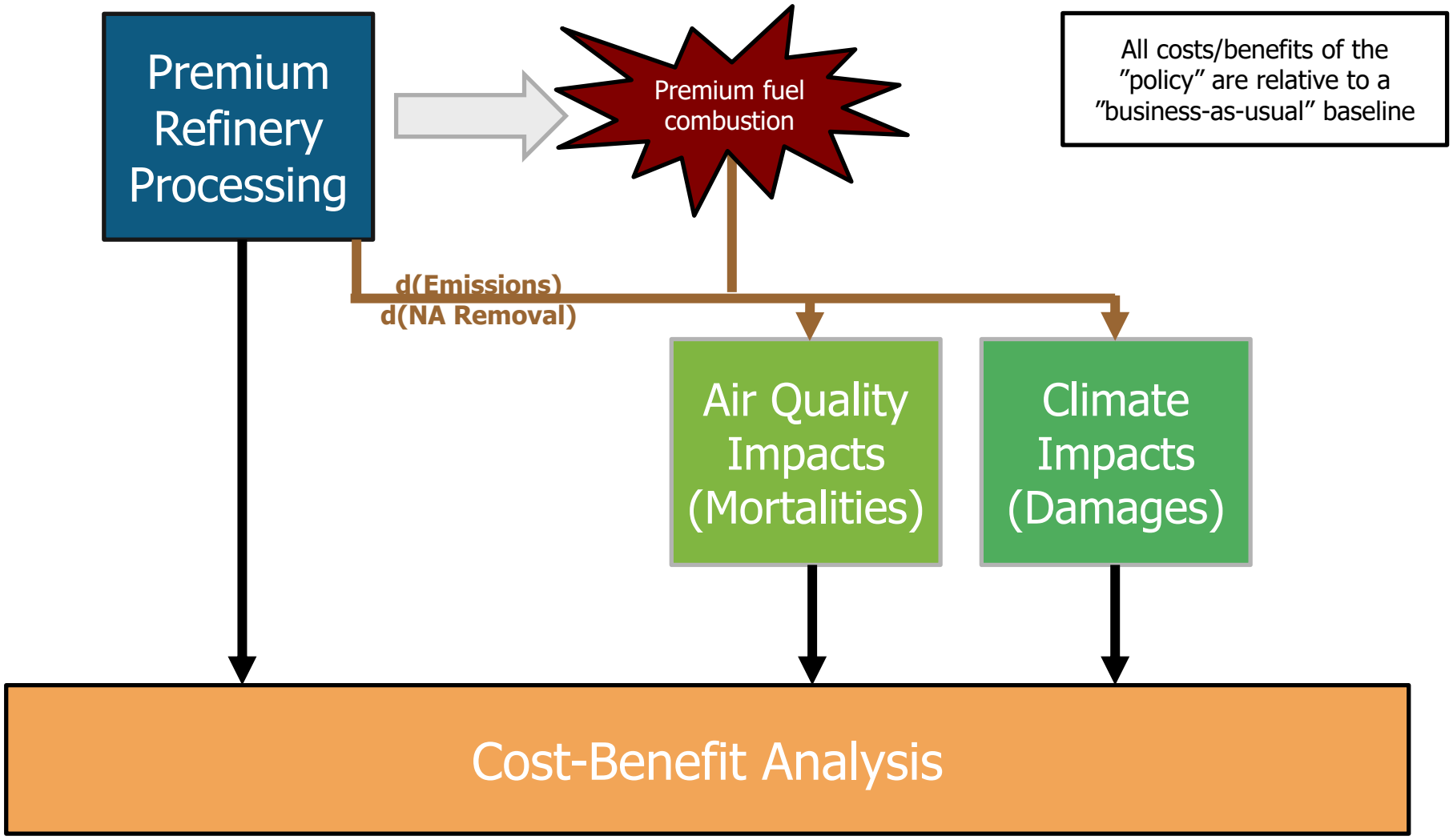
2b Near term objectives: Quantification of climate and AQ impacts

Radiative Source	Air Quality Impact	Climate Impact	Description
Reduced nvPM	**Reduced Mortality**	Cooling	Reduced soot emissions from jet engine tailpipe
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 Mortality	Warming	Reduced fuel sulfur content from refining

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

- Tools used for estimated climate / AQ impacts
  - Climate: **APMT-I Climate**
  - AQ: North American nested domain simulations using **GEOS-Chem** Chemistry Transport Model

2b Near term objectives: Integrated cost/benefit analysis



Summary

Summary

- A **U.S.-wide cost-benefit analysis** of Naphthalene Removal is desirable to inform future Jet-A standard policy.
  - Removal of jet fuel naphthalene has the potential to significantly reduce nvPM emissions, therefore reducing aviation's climate and AQ impacts
- Completed
  - **U.S. Societal Cost estimate** are 9.51¢/gal (8.73, 10.26) for hydro-treatment and 7.73 ¢/gal (6.81, 8.60) for extractive distillation
- Next Steps
  - **Detailed-chemistry chemical reactor network** used for nvPM estimation
  - Existing tools used to **estimate climate / AQ impacts**

References

J. H. Gary, G. E. Handwerk, and M. J. Kaiser, *Petroleum Refining: Technology and Economics, Fifth Edition*. CRC Press, 2007.

R. L. Speth, C. Rojo, R. Malina, and S. R. H. Barrett, "Black carbon emissions reductions from combustion of alternative jet fuels," *Atmospheric Environment*, vol. 105, pp. 37–42, Mar. 2015.

D. L. A. F. B. VA, "Petroleum Quality Information System 2013 Annual Report," Jan. 2013.

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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.

G. Hoek *et al.*, "Long-term air pollution exposure and cardio- respiratory mortality: a review," *Environmental Health*, vol. 12, p. 43, 2013.

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"GlobalData O&G," *Oil&Gas: Downstream Analytics*.

Contributors

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- Mengjie Liu
- Raymond Speth
- William Green
- Steven Barrett

BACK-UP SLIDES

1a Process 1: Hydro-treatment

- Refining process used for sulfur, nitrogen, and metal removal, and saturation of aromatics and olefins
- Feedstock is reacted, at mild temperatures (~360° C) and pressures (50–100 bar), with high-purity hydrogen

Relative Activity of Reaction Families
(Most Active → Least Active)

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Sulfur Removal + Olefin Saturation
Halogen + Oxygen Removal
Nitrogen Removal + Aromatic Saturation

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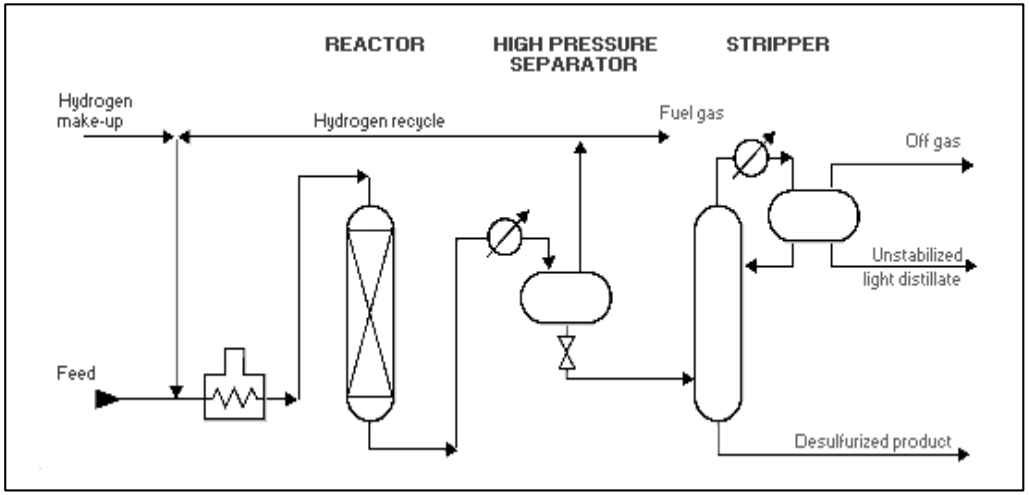
Hydrogen Consumption: 100 – 400 scfb[7]



1a Process 2: Extractive distillation

- Refining process by which the desired extract is separated from the feed via solution with a polar solvent
- Aromatic extract first separated from feed, then mono-aromatics and naphthalene's are separated via distillation

Relative Solubility of Components (Most Active → Least Active)

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Aromatics (Mono → Di)
S, N, O, Halogen impurities
Naphthenes / Cycloalkanes
Alkanes

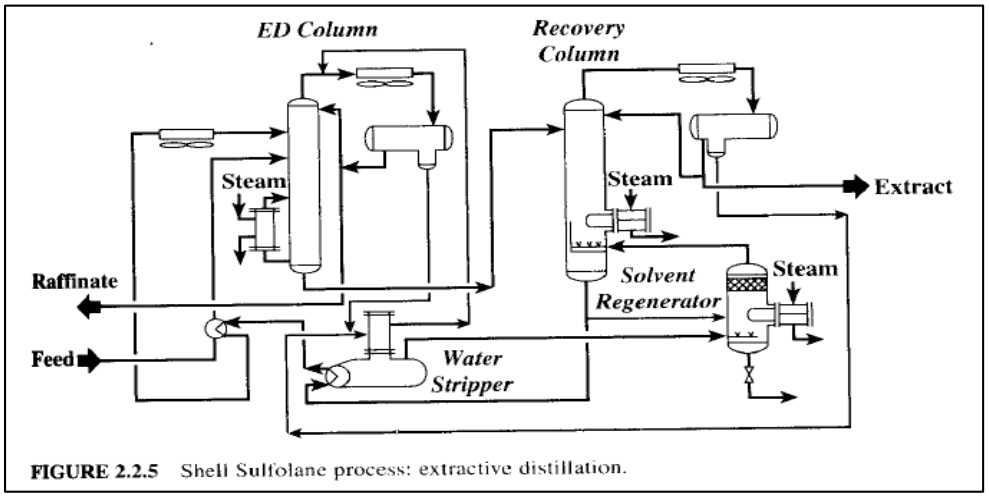

FIGURE 2.2.5 Shell Sulfolane process: extractive distillation.