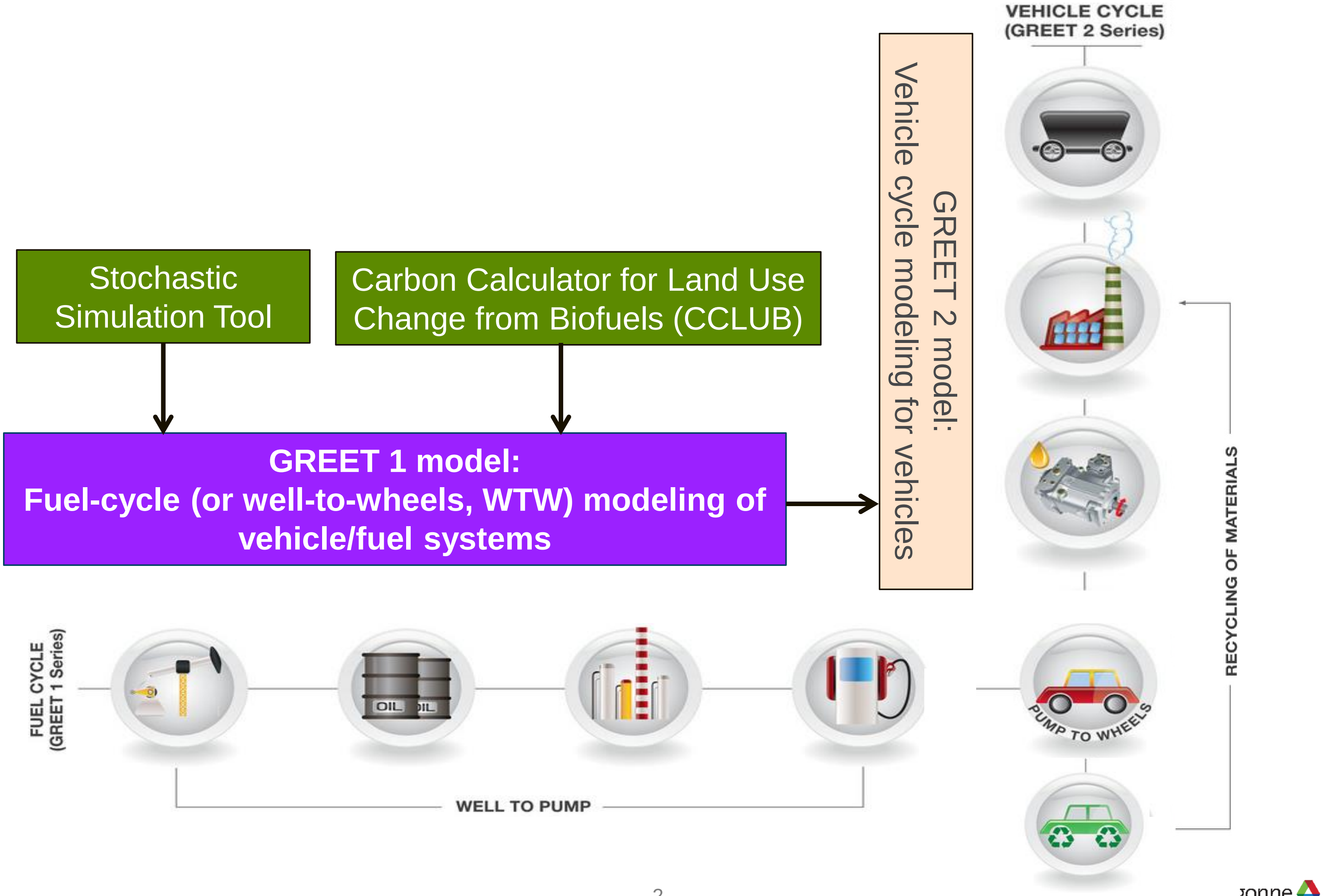
THE LIFE-CYCLE ANALYSIS OF PETROLEUM FUELS AND BIOFUELS WITH GREET®

MICHAEL WANG, JEONGWOO HAN, AMGAD ELGOWAINY

Systems Assessment Group
Energy Systems Division
Argonne National Laboratory

CARB LCFS Team Evaluation of Co-Processing of Crude and Bio-feedstocks
Sacramento, CA, Dec. 13, 2016

The GREET® (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model



Stochastic Simulation Tool

Carbon Calculator for Land Use Change from Biofuels (CCLUB)

GREET 1 model:
Fuel-cycle (or well-to-wheels, WTW) modeling of vehicle/fuel systems

GREET 2 model:
Vehicle cycle modeling for vehicles

GREET includes more than 100 fuel production pathways from various energy feedstock sources

Feedstock	Fuel
Petroleum Conventional crude Shale oil Oil Sands	Gasoline Diesel Jet Fuel Liquefied Petroleum Gas Naphtha Residual Oil
Coal Surface mining Underground mining	Hydrogen Fischer-Tropsch Diesel Fischer-Tropsch Jet Fuel Methanol Dimethyl Ether
Natural Gas North American Non-North American Shale gas	Compressed Natural Gas Liquefied Natural Gas Liquefied Petroleum Gas Methanol Dimethyl Ether Fischer-Tropsch Diesel Fischer-Tropsch Jet Fuel Fischer-Tropsch Naphtha Hydrogen
Renewable Natural Gas Landfill Gas Animal Waste Waste water treatment	
Coke Oven Gas Petroleum Coke Nuclear Energy Electricity from different sources	**Hydrogen**

Feedstock	Fuel
Corn	Ethanol Butanol Jet fuel
Sugarcane	Ethanol Jet Fuel
Soybeans Palm Rapeseed Jatropha Camelina Algae	Biodiesel Renewable Diesel Renewable Gasoline Renewable Jet Fuel
Cellulosic Biomass Switchgrass Willow/Poplar Crop Residues Forest Residues Miscanthus	Ethanol Hydrogen Methanol Dimethyl Ether Fischer-Tropsch Diesel Fischer-Tropsch Jet Fuel Pyro Gasoline/Diesel/Jet
Residual Oil Coal Natural Gas Nuclear Biomass Other Renewables	**Electricity**

GREET outputs include energy use, greenhouse gases, criteria pollutants and water consumption for vehicle and energy systems

- ☐ **Energy use**
  - ➢ Total energy: fossil energy and renewable energy
    - Fossil energy: petroleum, natural gas, and coal (they are estimated separately)
    - Renewable energy: biomass, nuclear energy, hydro-power, wind power, and solar energy

- ☐ **Greenhouse gases (GHGs)**
  - ➢ $CO_{2,}$ $CH_{4,}$ N_2O, black carbon, and albedo
  - ➢ CO_{2e} of the five (with their global warming potentials)

- ☐ **Air pollutants**
  - ➢ VOC, CO, $NO_{x,}$ $PM_{10,}$ $PM_{2.5,}$ and SO_x
  - ➢ They are estimated separately for
    - Total (emissions everywhere)
    - Urban (a subset of the total)

- ☐ **Water consumption**

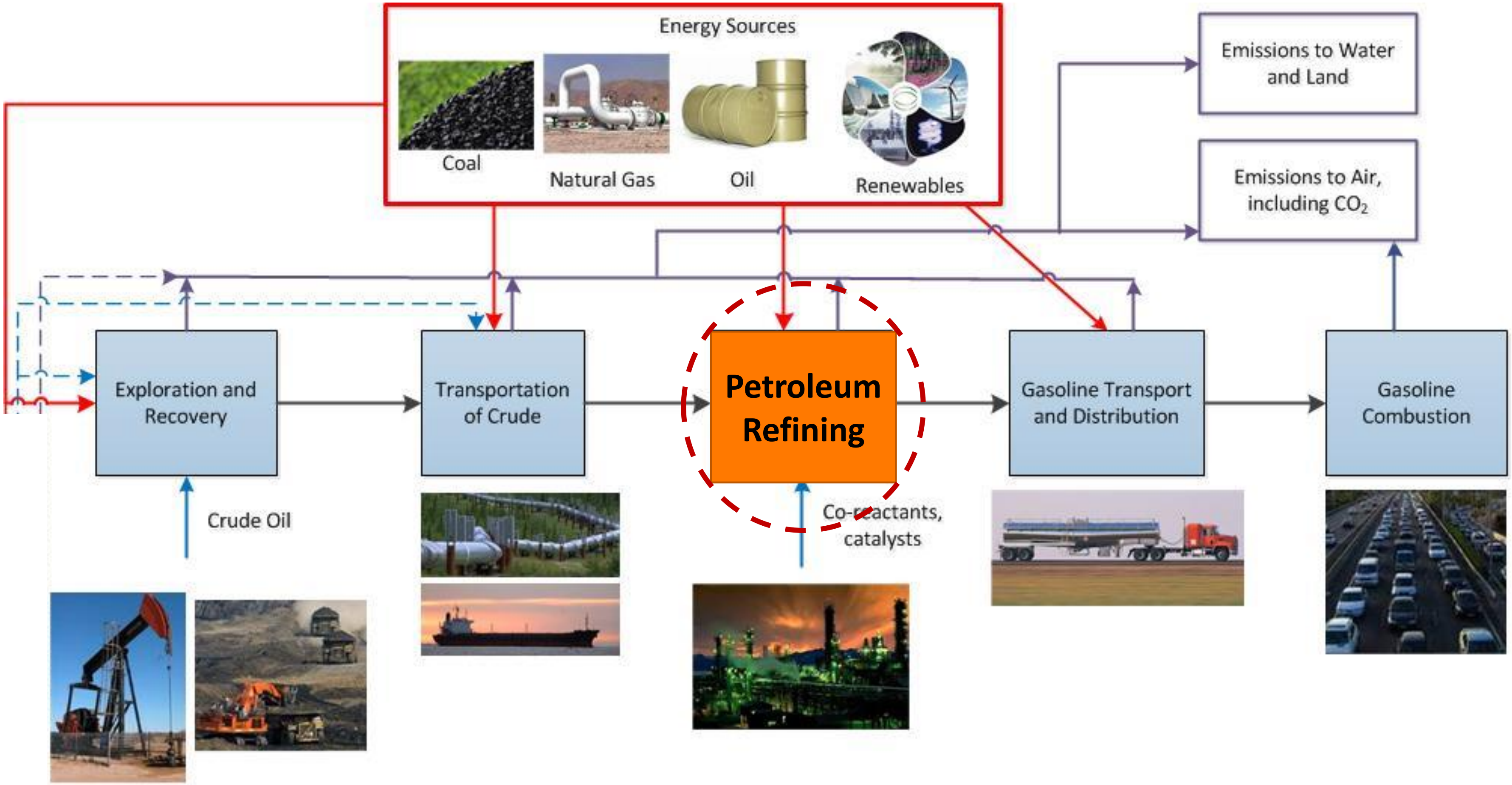
- ☐ **GREET LCA functional units**
  - ➢ Per service unit (e.g., mile driven, ton-mi)
  - ➢ Per unit of output (e.g., million Btu, MJ, gasoline gallon equivalent)
  - ➢ Per units of resource (e.g., per ton of biomass)

GREET data sources and ANL interactions with others

❑ Data are key to GREET reliability

- ➢ Open literature and results from other researchers
- ➢ Baseline technologies and energy systems: EIA AEO projections, EPA eGrid for electric systems, etc.
- ➢ Consideration of effects of regulations already adopted by agencies
- ➢ Fuel production processes (WTP)
  - ANL simulations with chemical processing models such as ASPEN Plus
  - Interactions with energy companies via US DRIVE
  - Interactions with new fuel producers
- ➢ Vehicle operations (PTW)
  - ANL Autonomie team modeling results for DOE VTO/FCTO and US DRIVE
  - OEM research results and interactions via US DRIVE
  - EPA MOVES and other models

WTW analysis of petroleum fuels pathways



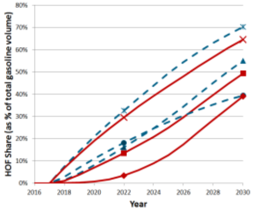
Refining process

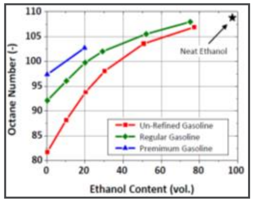
- ✓ Second-largest GHG emissions source in petroleum fuel cycle
- ✓ Complex system with multiple co-products

Refinery LP modeling is a key part of LCA of petroleum products

Crude Slate

Product Slate

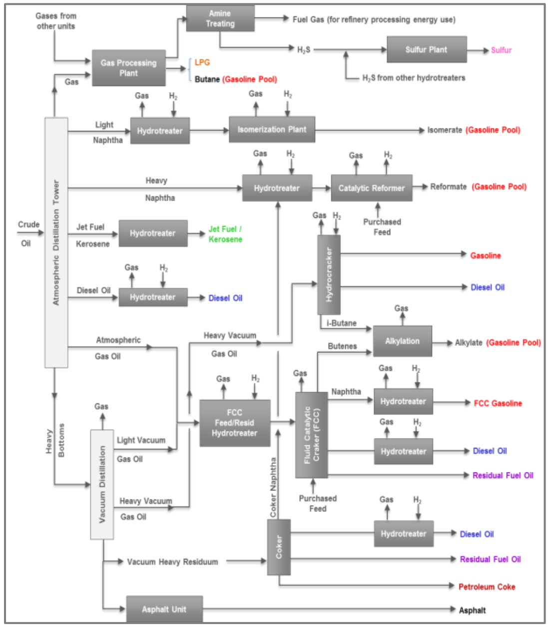




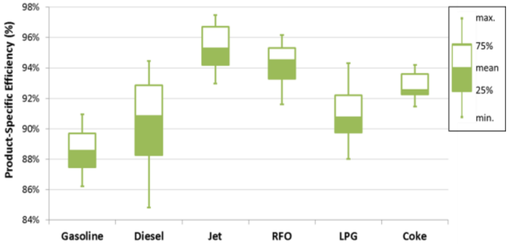
Fuel Specifications (RON, RVP)

Economic factors

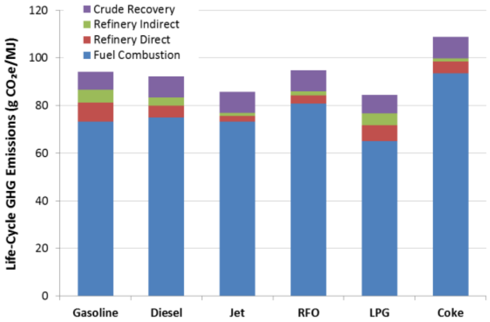
Refinery LP Modeling



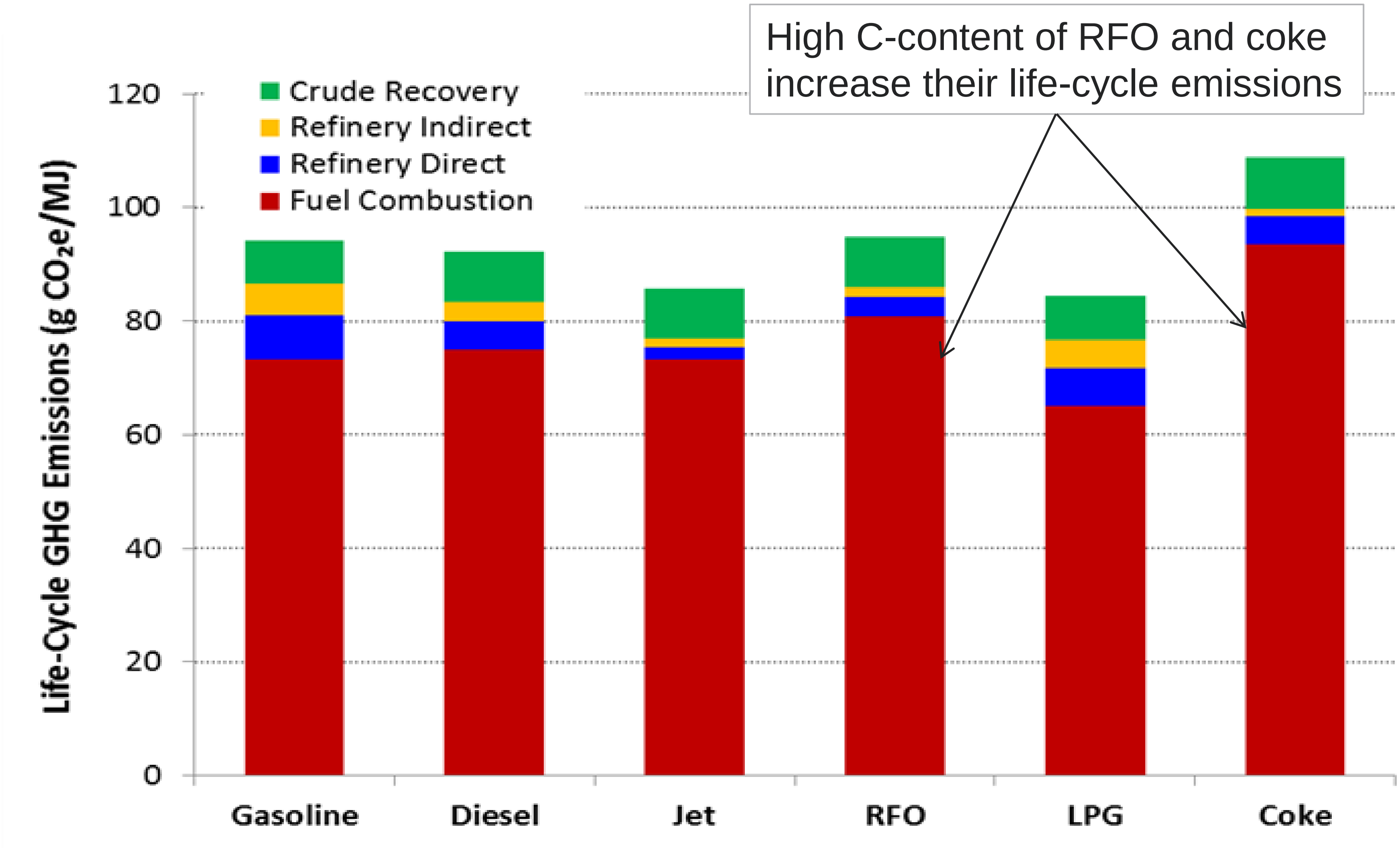
Refining Efficiency



Life-Cycle Analysis

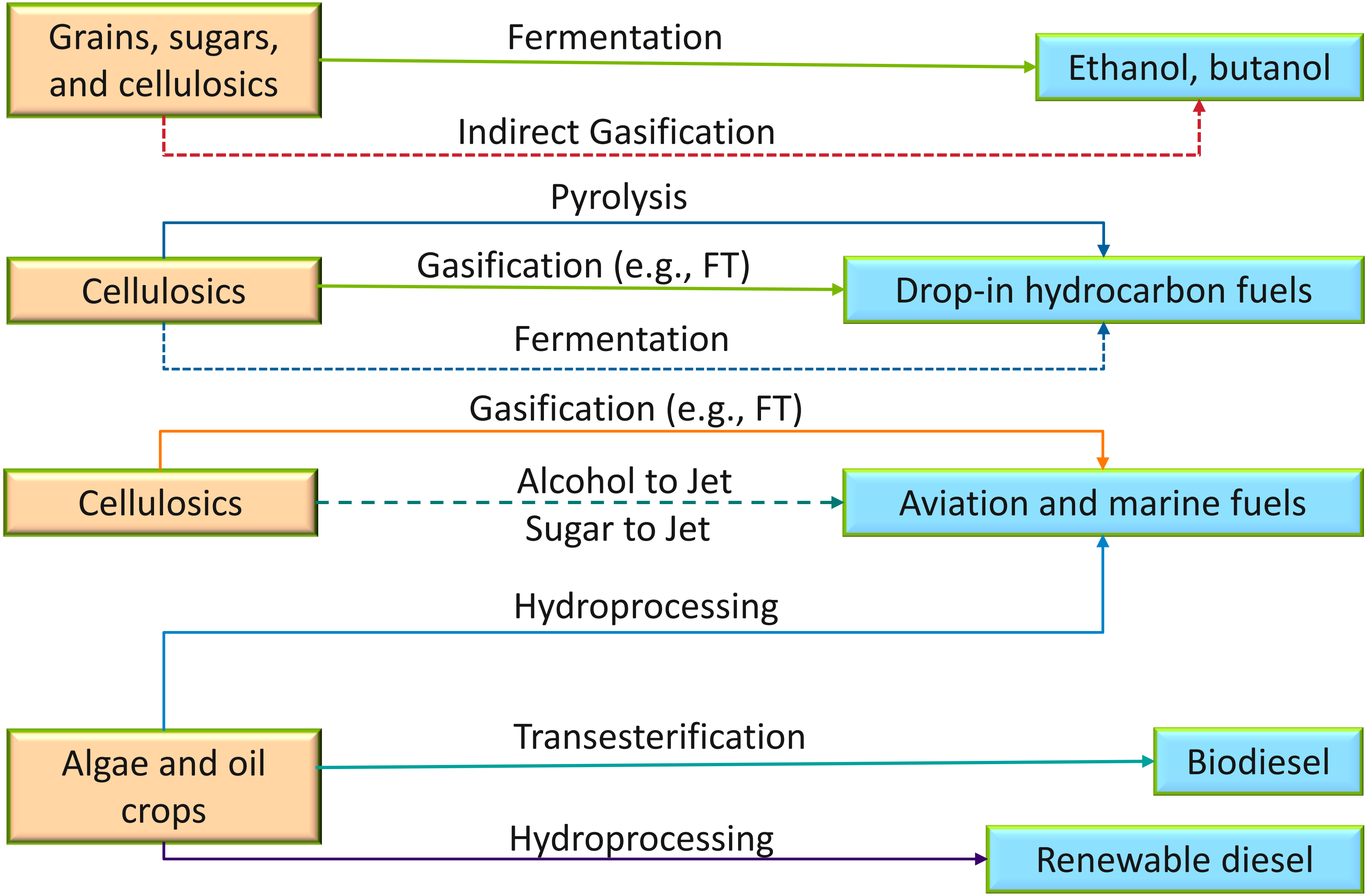


LCA GHG emissions of petroleum fuels are dominated by end-use release of CO2; refinery emissions is a distant second



High C-content of RFO and coke increase their life-cycle emissions

GREET includes various biomass feedstocks, conversion technologies, and liquid fuels



Grains, sugars, and cellulosics

Fermentation

Ethanol, butanol

Indirect Gasification

Pyrolysis

Cellulosics

Gasification (e.g., FT)

Drop-in hydrocarbon fuels

Fermentation

Gasification (e.g., FT)

Cellulosics

Alcohol to Jet

Sugar to Jet

Aviation and marine fuels

Hydroprocessing

Algae and oil crops

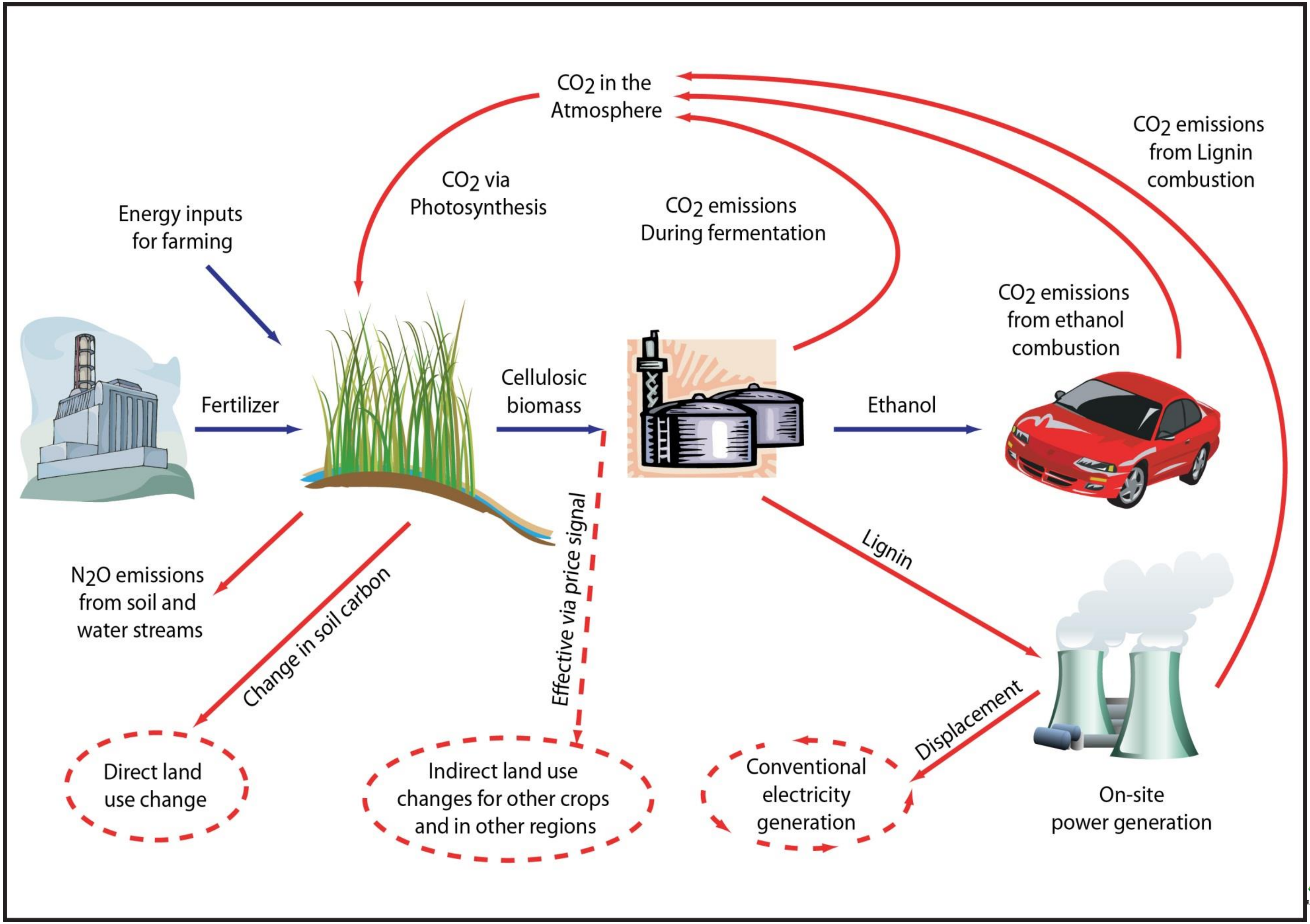
Transesterification

Biodiesel

Hydroprocessing

Renewable diesel

LCA system boundary: switchgrass to ethanol



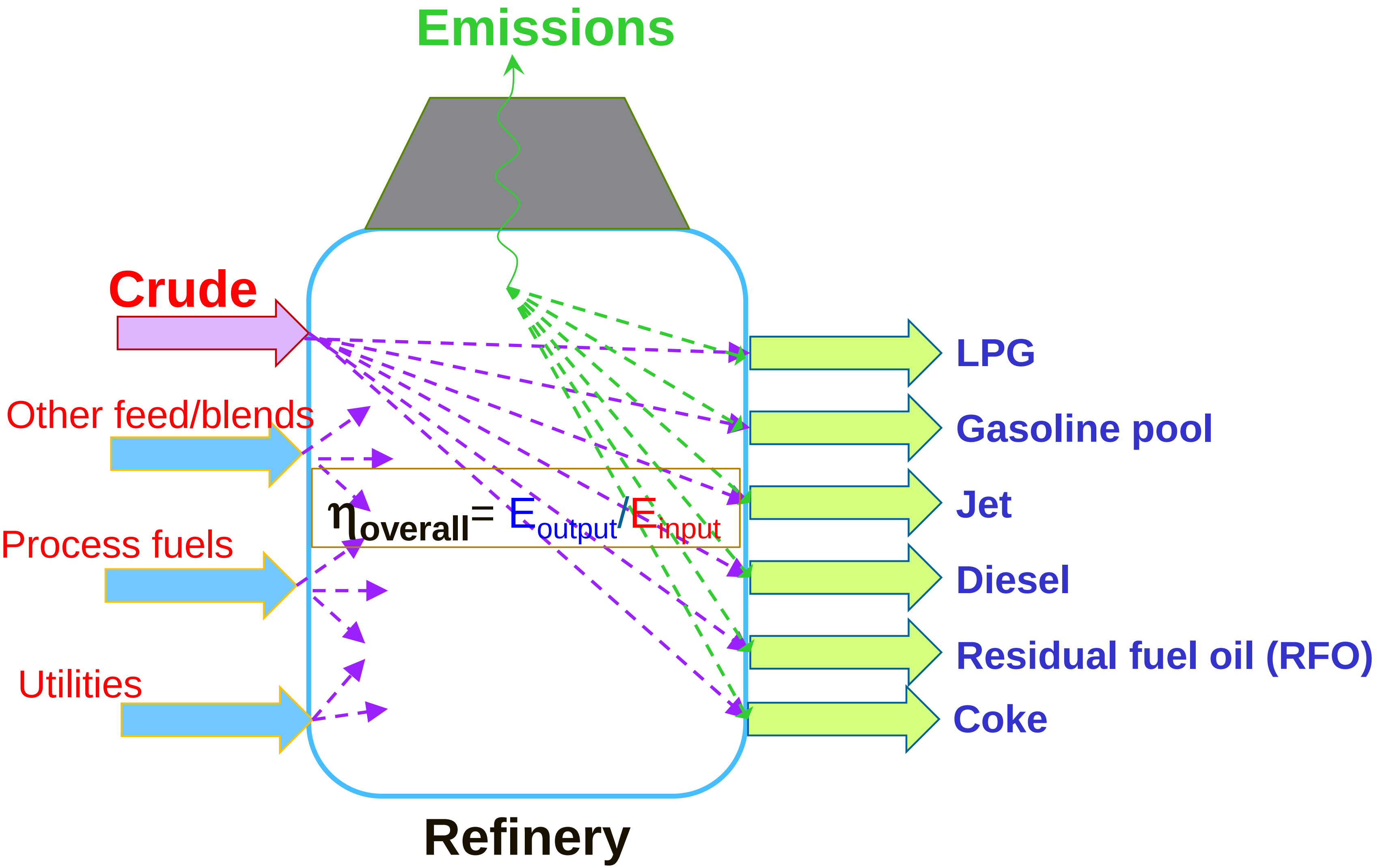
ANL LP MODELING OF U.S. INDIVIDUAL REFINERIES

-- Petroleum product efficiencies

-- Co-product methods for refineries

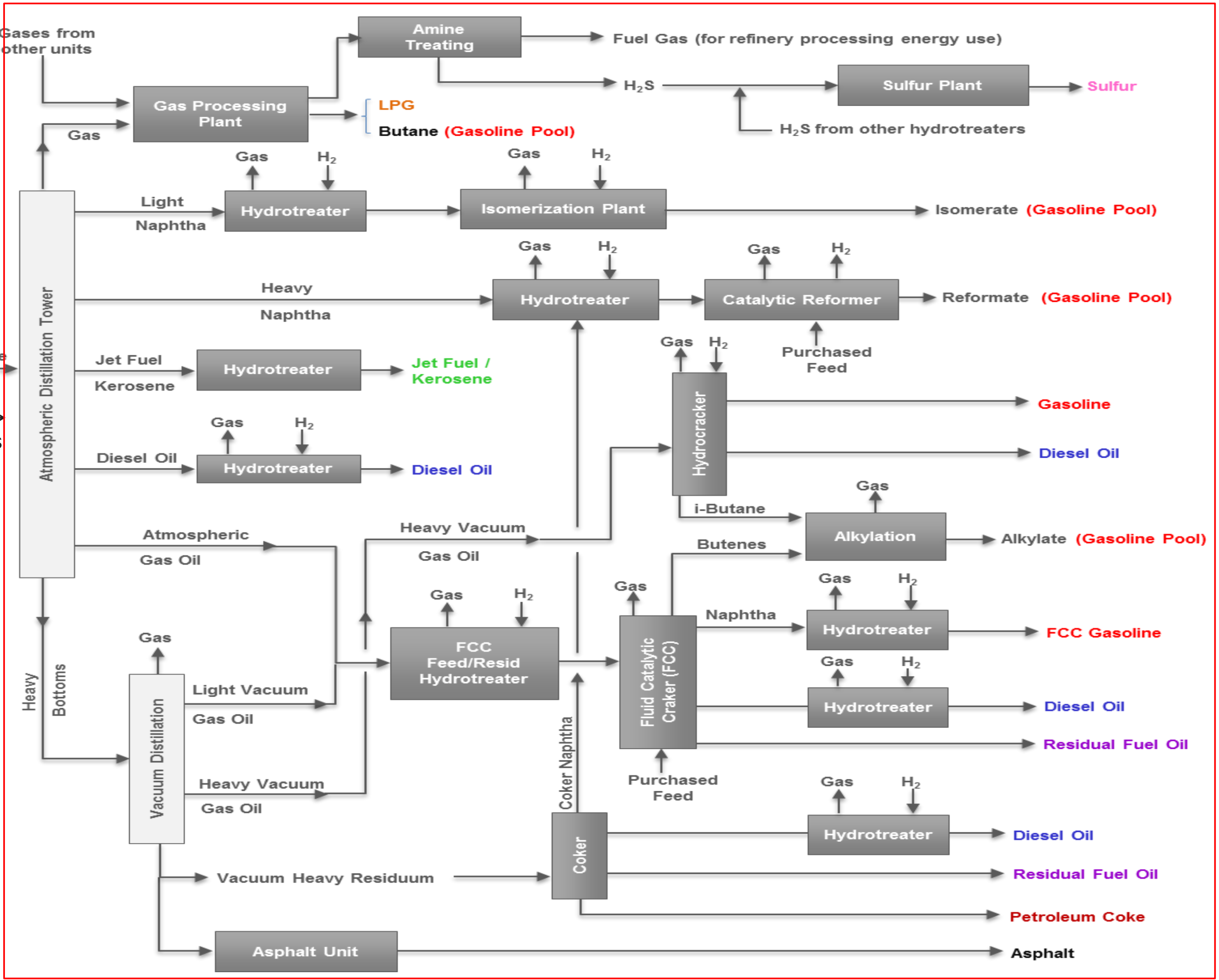
-- Three journal articles

Determining of overall refinery efficiency and product-specific energy and GHG emission intensity



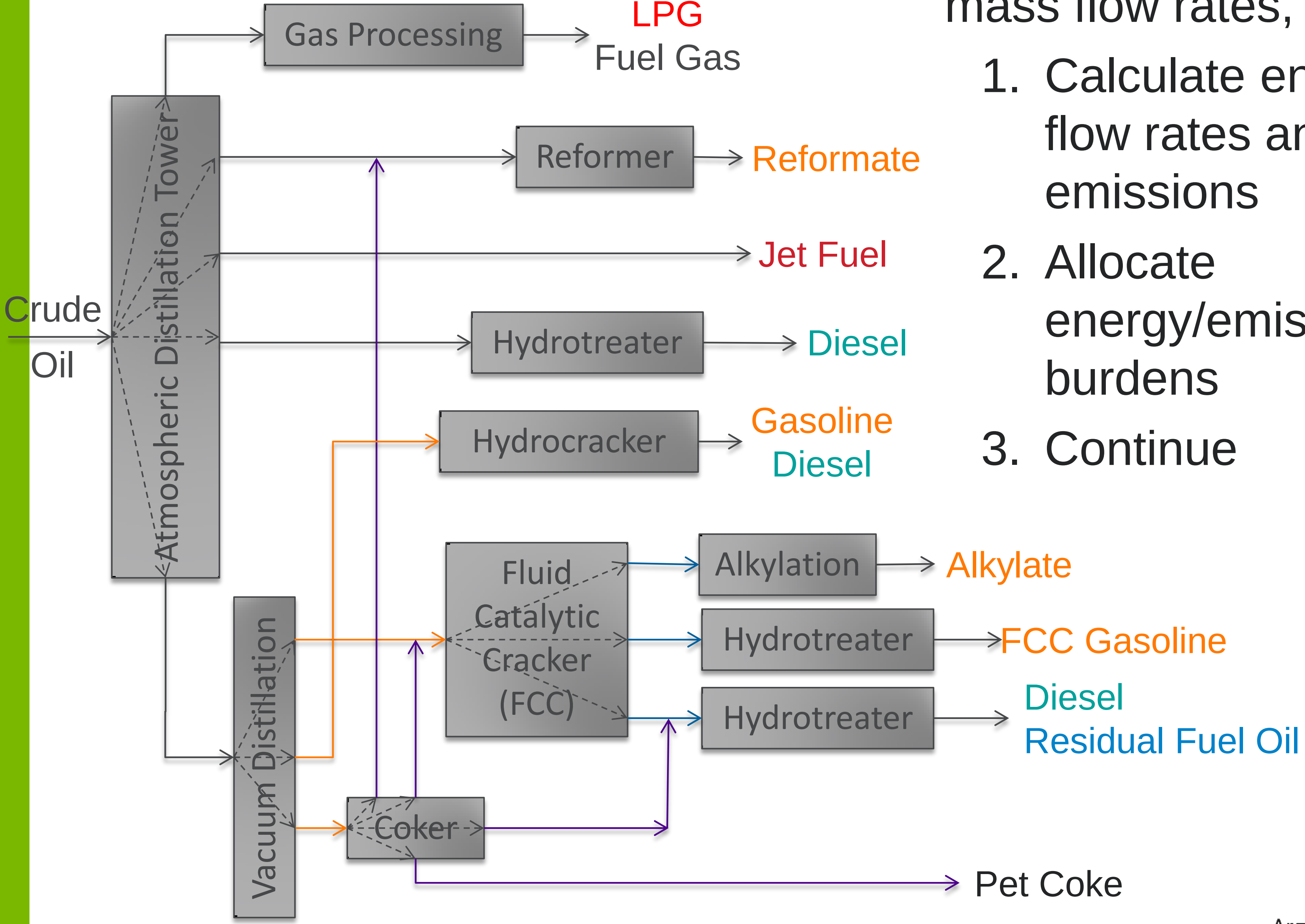
$\eta_{overall} = E_{output} / E_{input}$

Process mass and energy balance data are key for proper allocation of energy and emission burden to refinery products



-Other feed/blends
-Process fuels
-Utilities

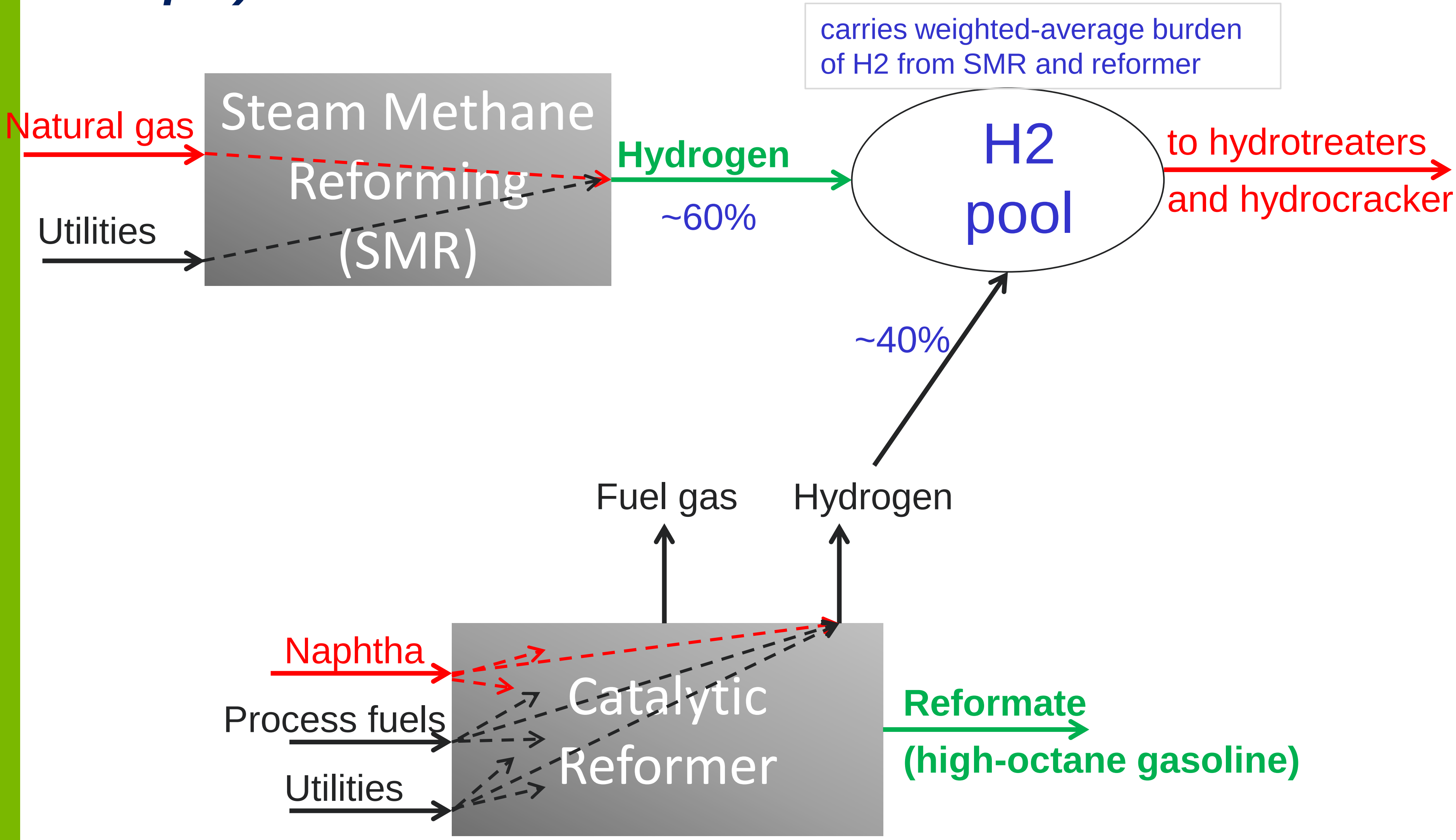
Process-level allocation



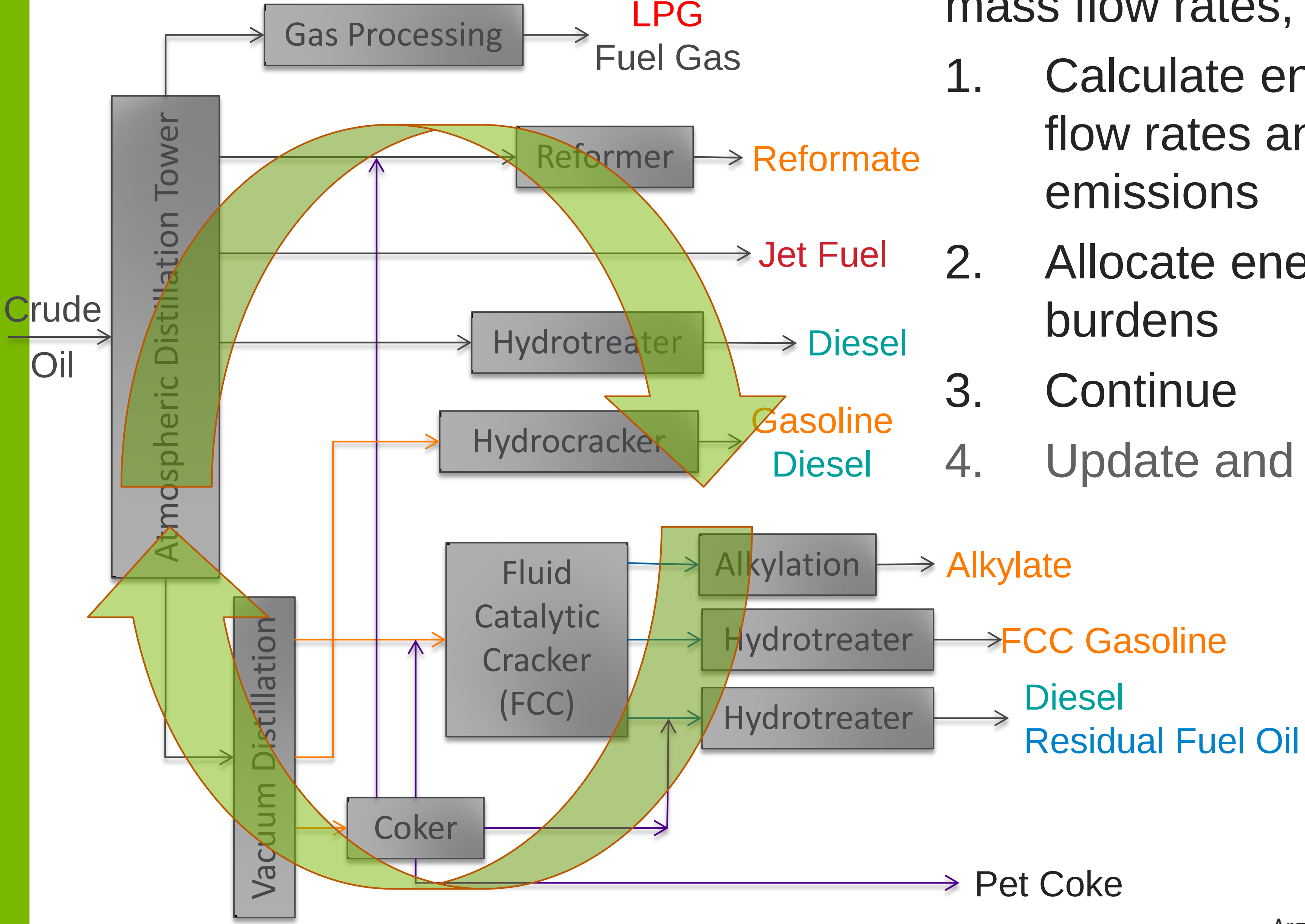
Given volumetric and mass flow rates,

1. Calculate energy flow rates and emissions
2. Allocate energy/emission burdens
3. Continue

Allocation methodology of energy between products at process-unit level to make product pools (H2 pool as example)



Process-level allocation



Given volumetric and mass flow rates,

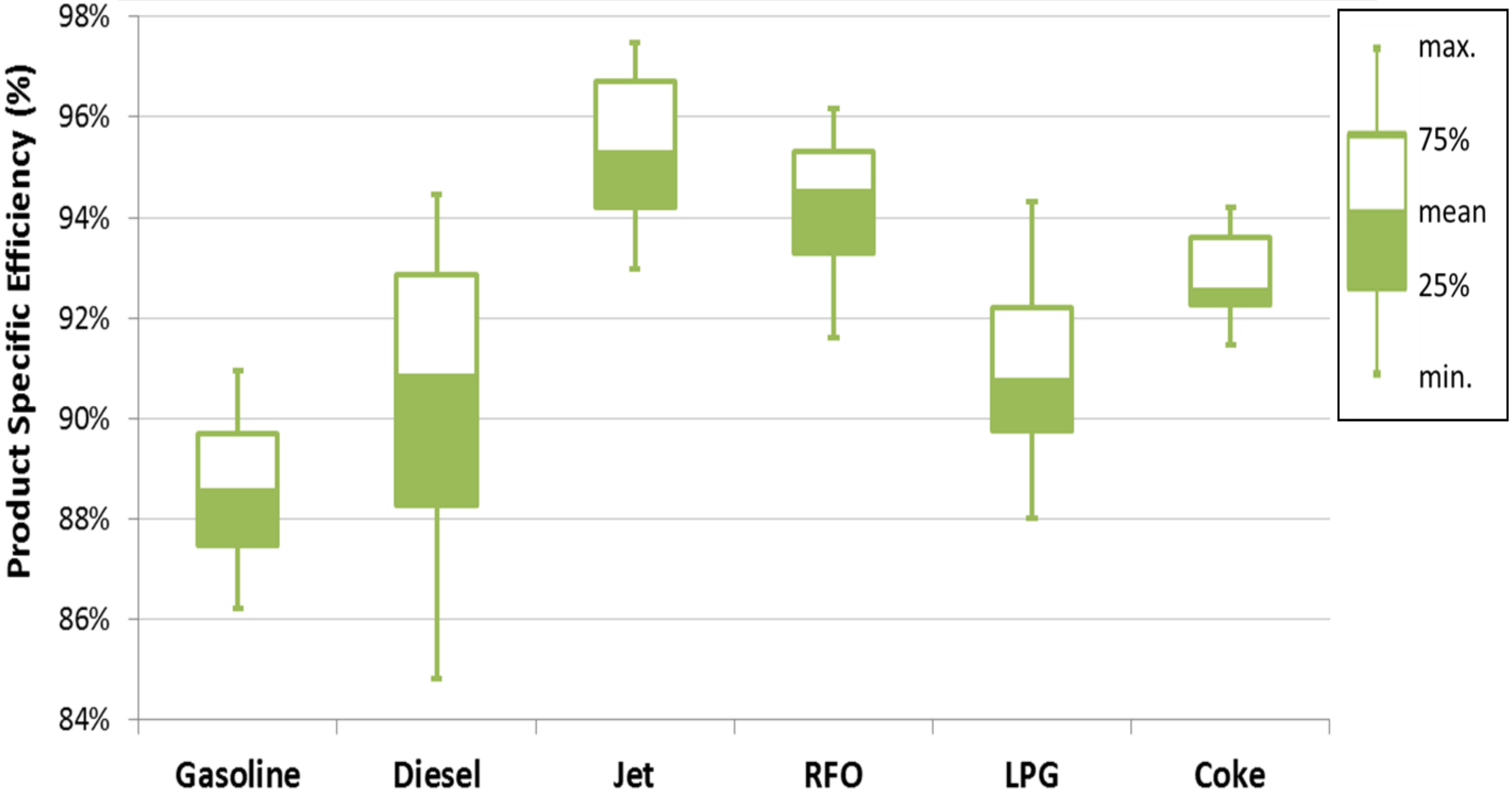
1. Calculate energy flow rates and emissions
2. Allocate energy burdens
3. Continue
4. Update and iterate

Key challenges in process-level allocation

- ☐ Data Size
  - ➢ Dozens of process units and hundreds of intermediate streams in a refinery
- ☐ Variations in Refinery
  - ➢ Configurations
    - ✓ Topping, Hydroskimming, Cracking, Light Coking, and Heavy Coking
  - ➢ Operations by fuel specifications, region, season, economic conditions, etc.
- ☐ Developed an algorithm to automate the processing of data
  - ➢ Implemented validation procedures to ensure accuracy
  - ➢ Analyzed 60 large refineries in the U.S. and Europe

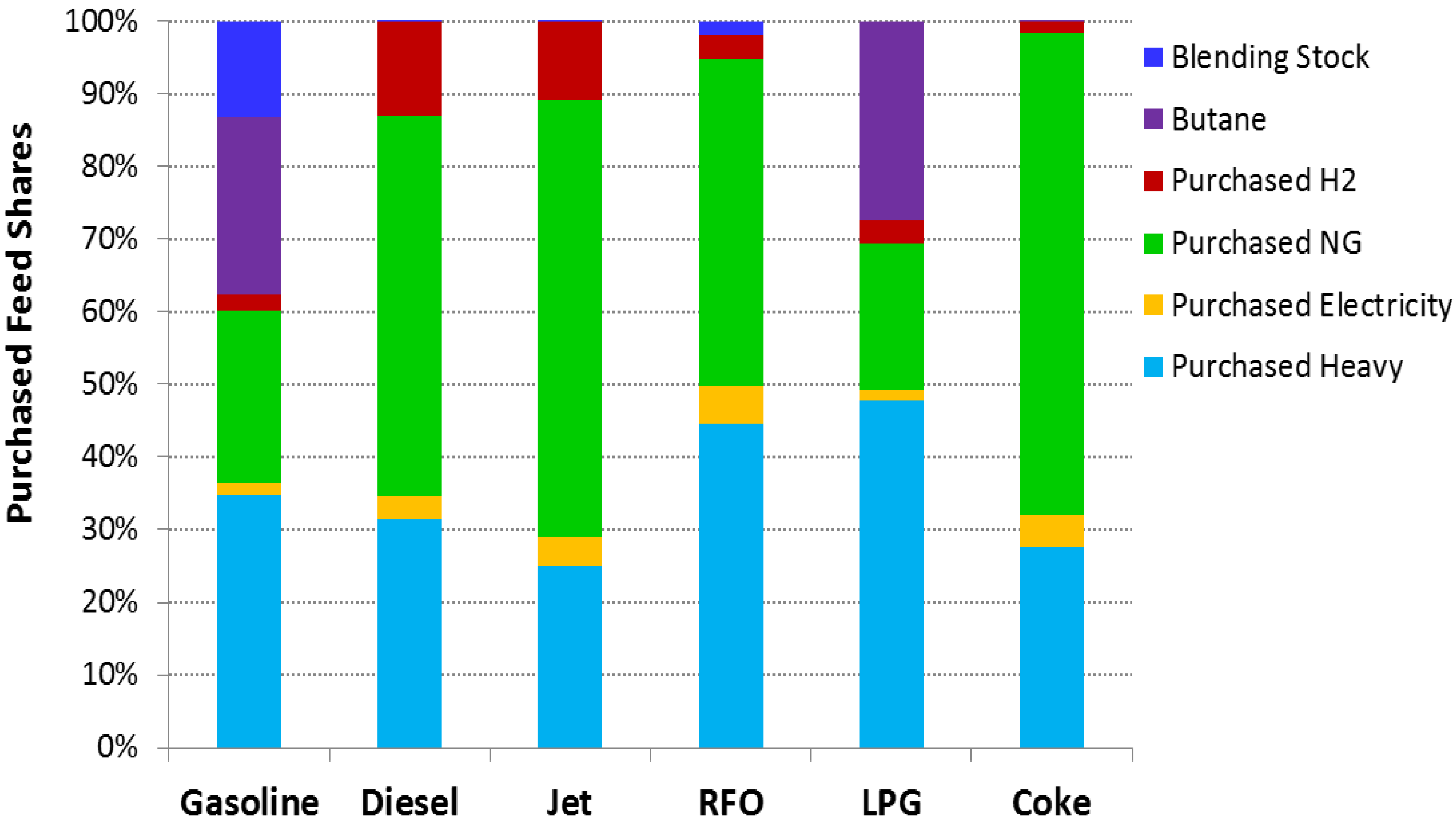
Product-specific efficiency reflects the energy intensity of the refining units contributing to each product pool

- Refining unit contributions to each pool vary among 43 refineries
- Wider efficiency range for diesel compared to other products

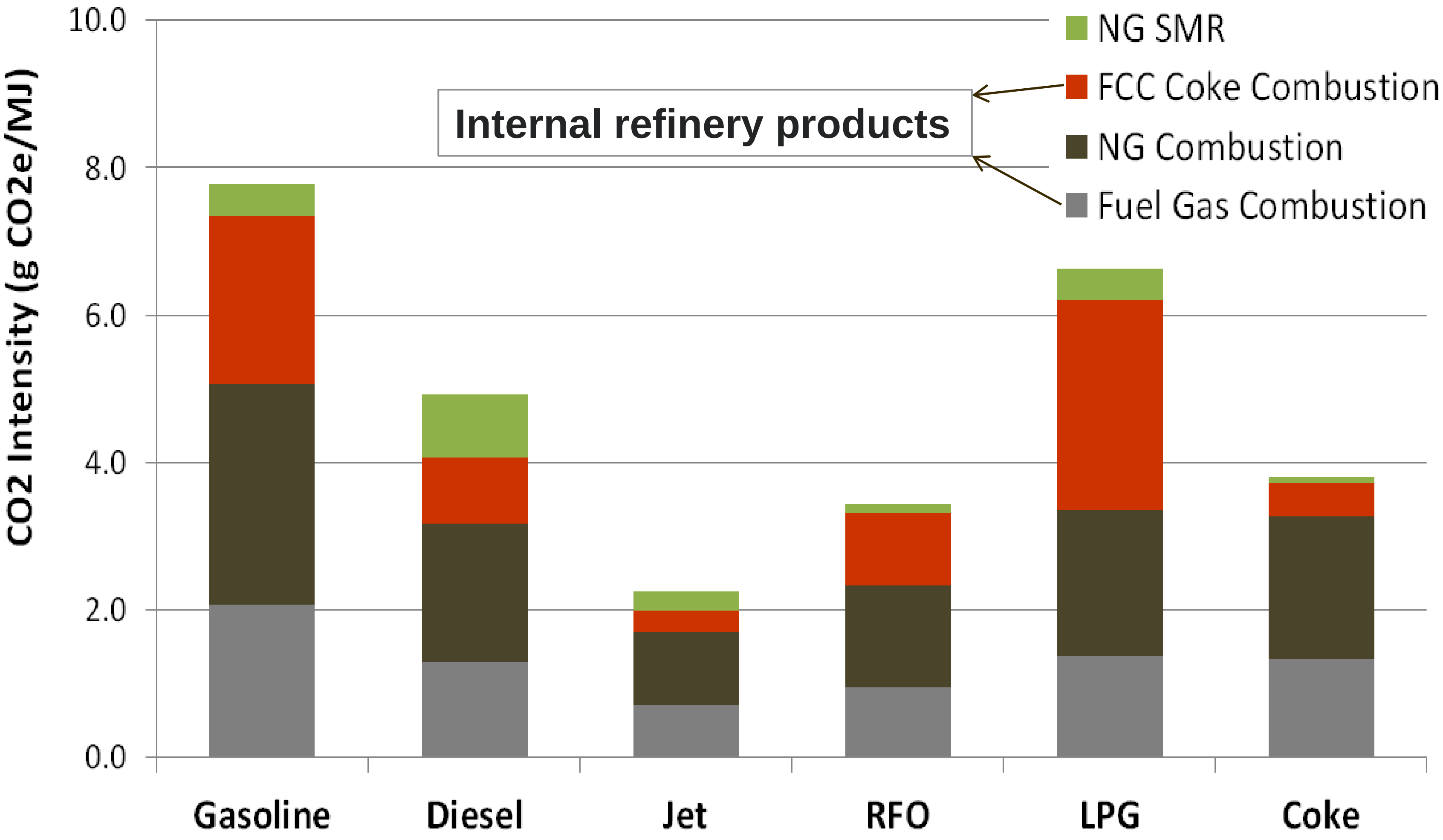


Process-unit data allows the distribution of energy in purchased feed/fuel/utility shares to major refinery products

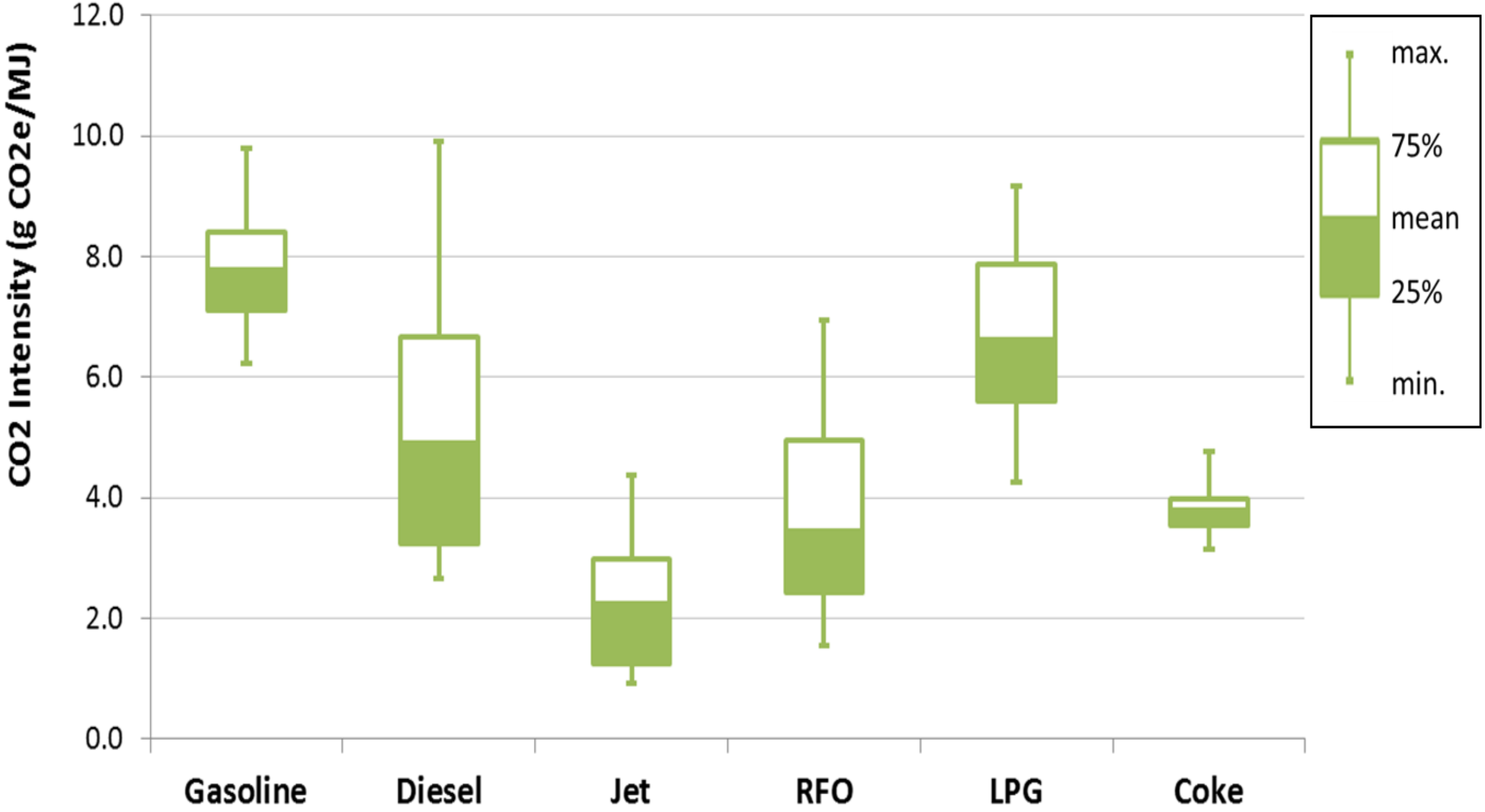
- Need process fuel shares to calculate carbon intensity of each refinery product



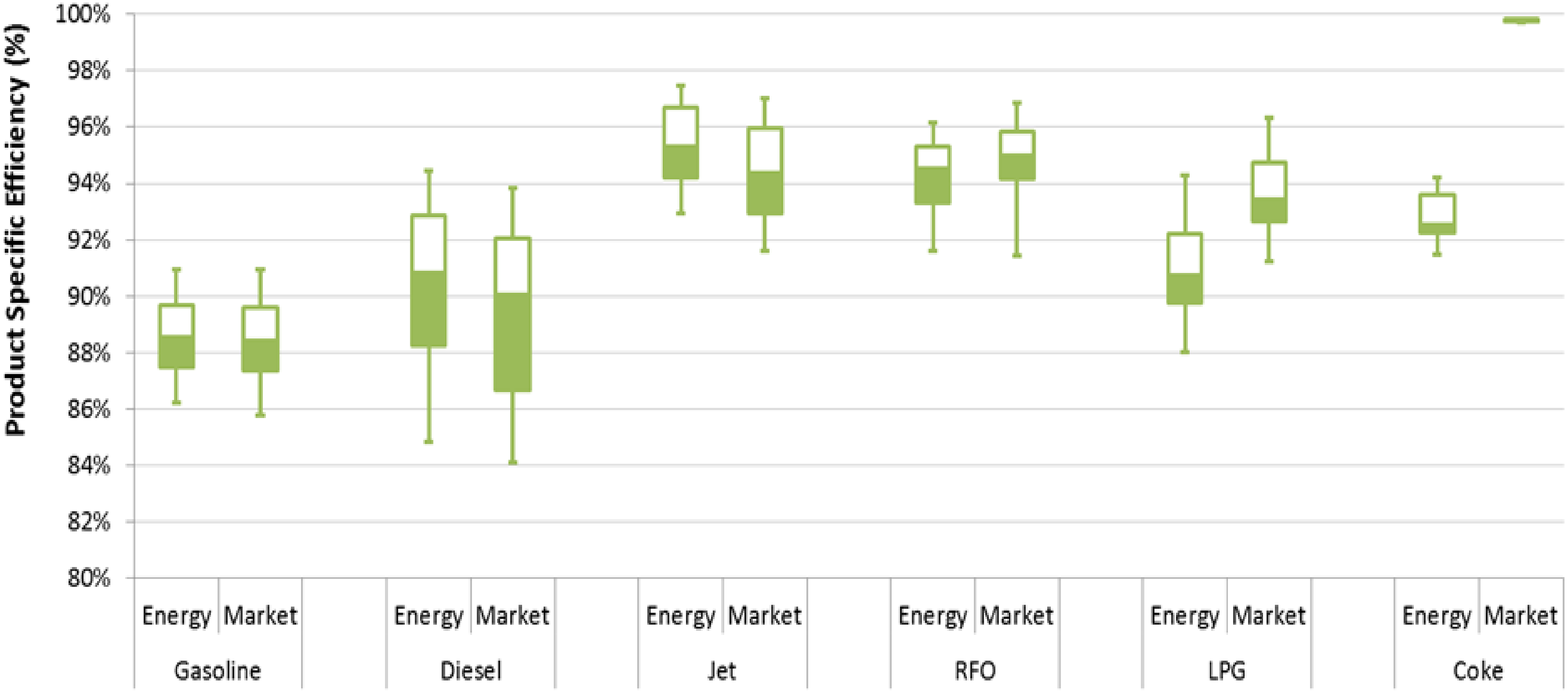
FCC coke, NG and fuel gas combustion are the major contributors to refinery products CO_2 intensity



Range of CO2 intensity reflects the contribution of various refining units and their process fuel types to each product pool in the 43 U.S. refineries



Impact of allocation metric on efficiencies: only LPG and coke are affected noticeably



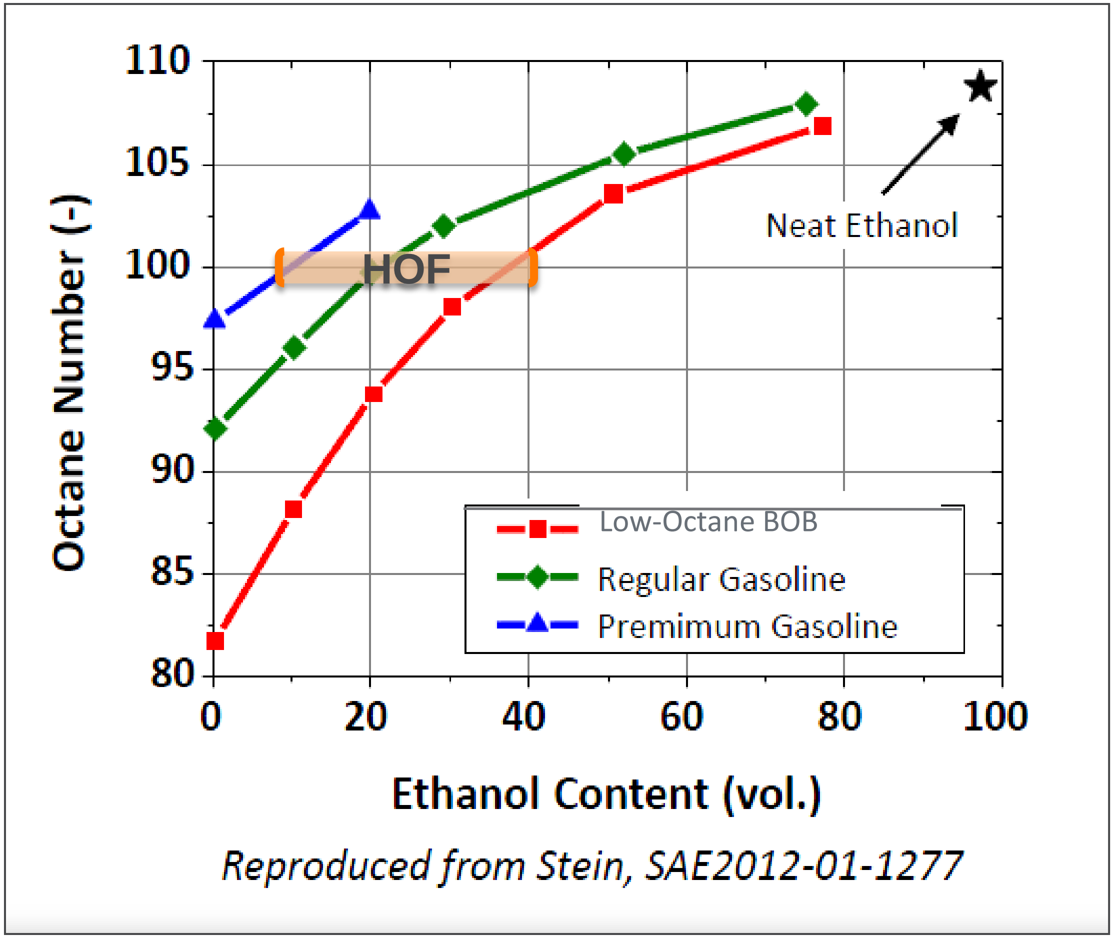
ANL LP MODELING OF HIGH OCTANE FUEL (HOF) PRODUCTION:

-- Impacts of ethanol blending on refinery operation and efficiency

-- two peer-reviewed reports

Motivation for high-octane fuels

- Higher octane allows for more aggressive engine design, which can improve efficiency
- Non-linear effects of ethanol content
- Non-linear benefit of higher octane vs. linear decrease in energy density

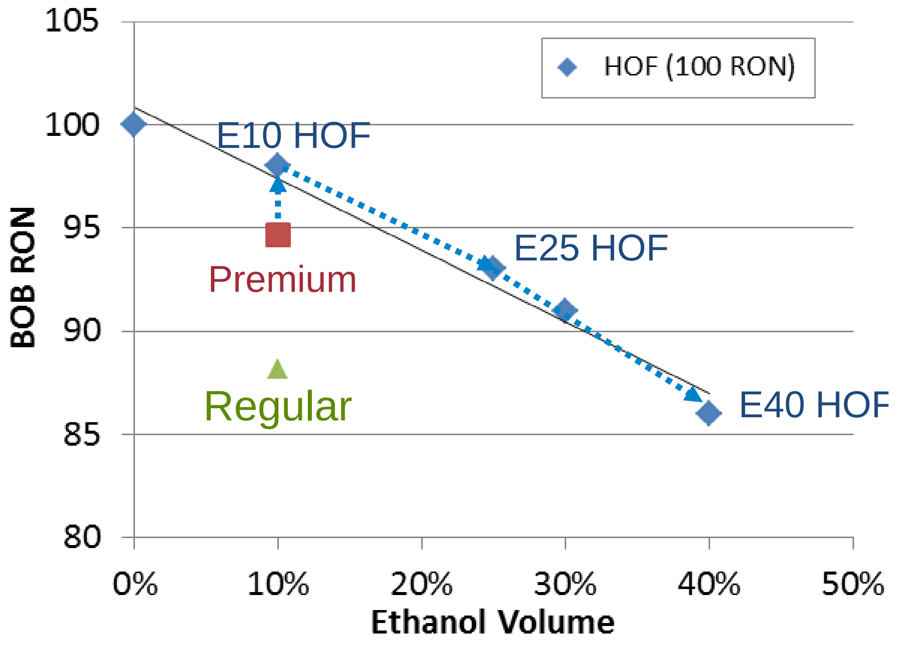


Reproduced from Stein, SAE2012-01-1277

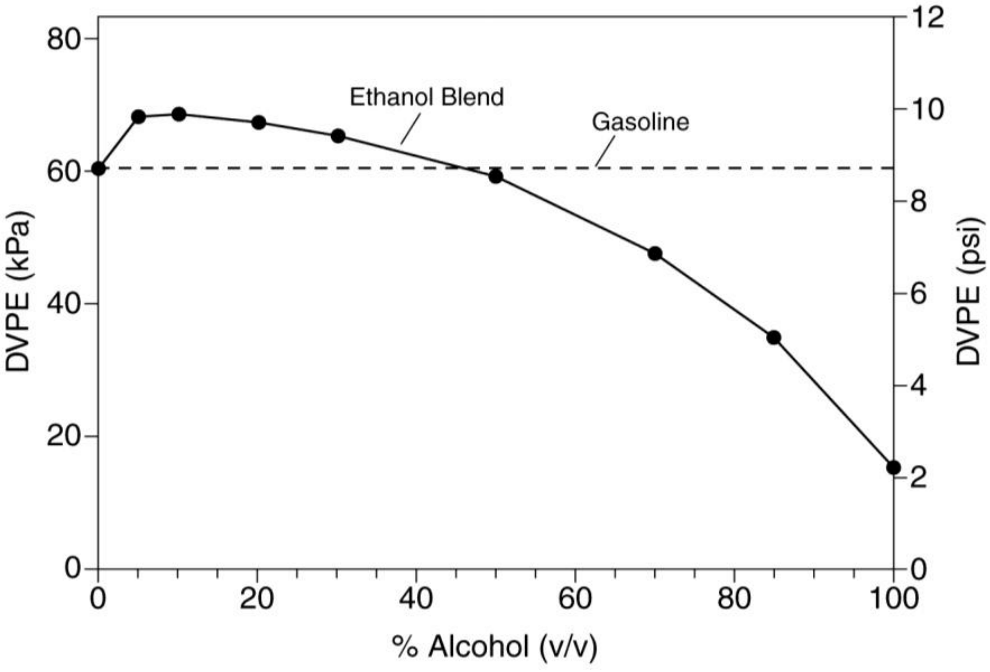
Define "High Octane Fuel" (HOF) as RON ~ 100

Research Octane Number (RON) and Reid Vapor Pressure (RVP) are key fuel specifications for refineries

BOB RON vs. Ethanol Volume Share

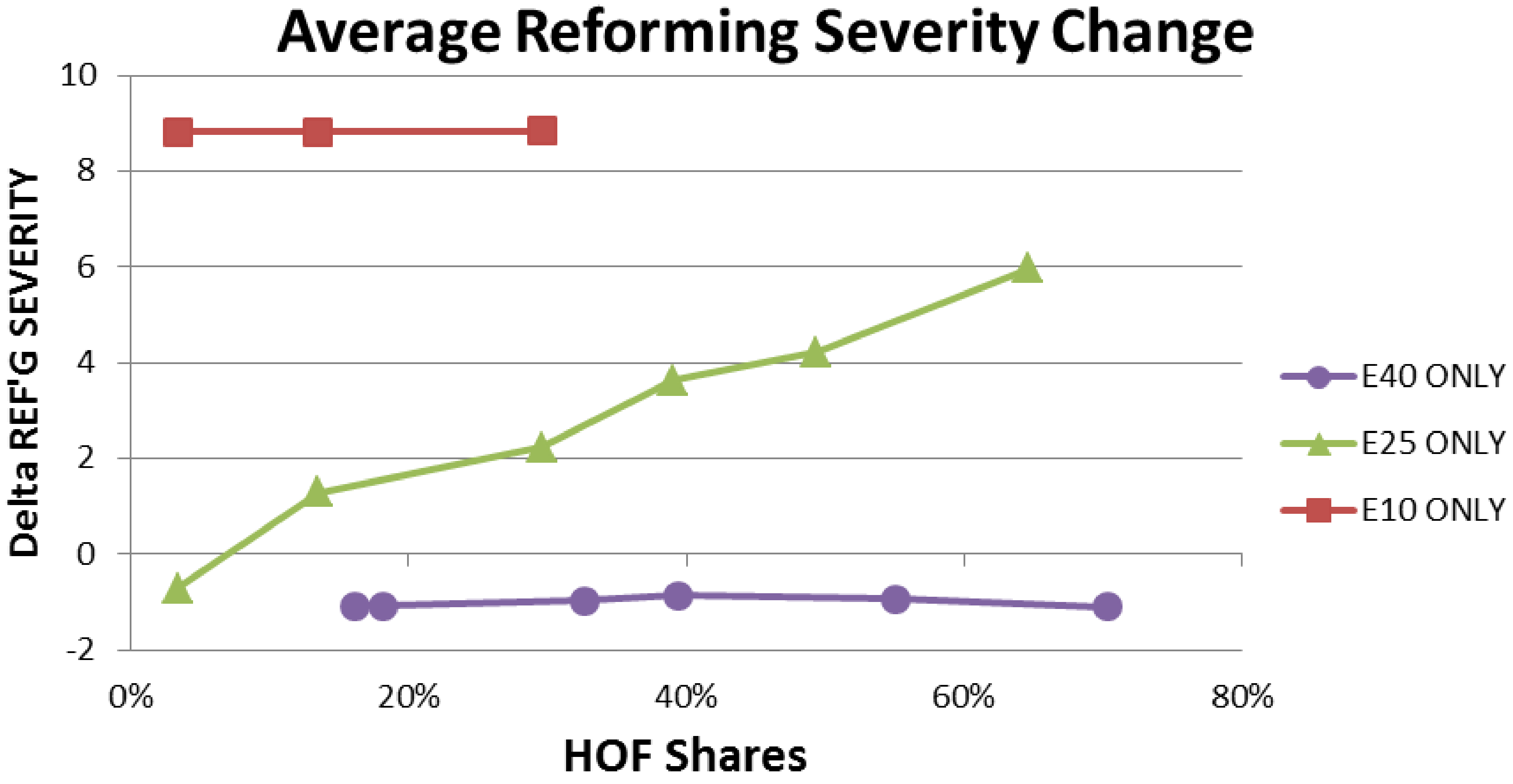


RVP vs. Ethanol Volume Share



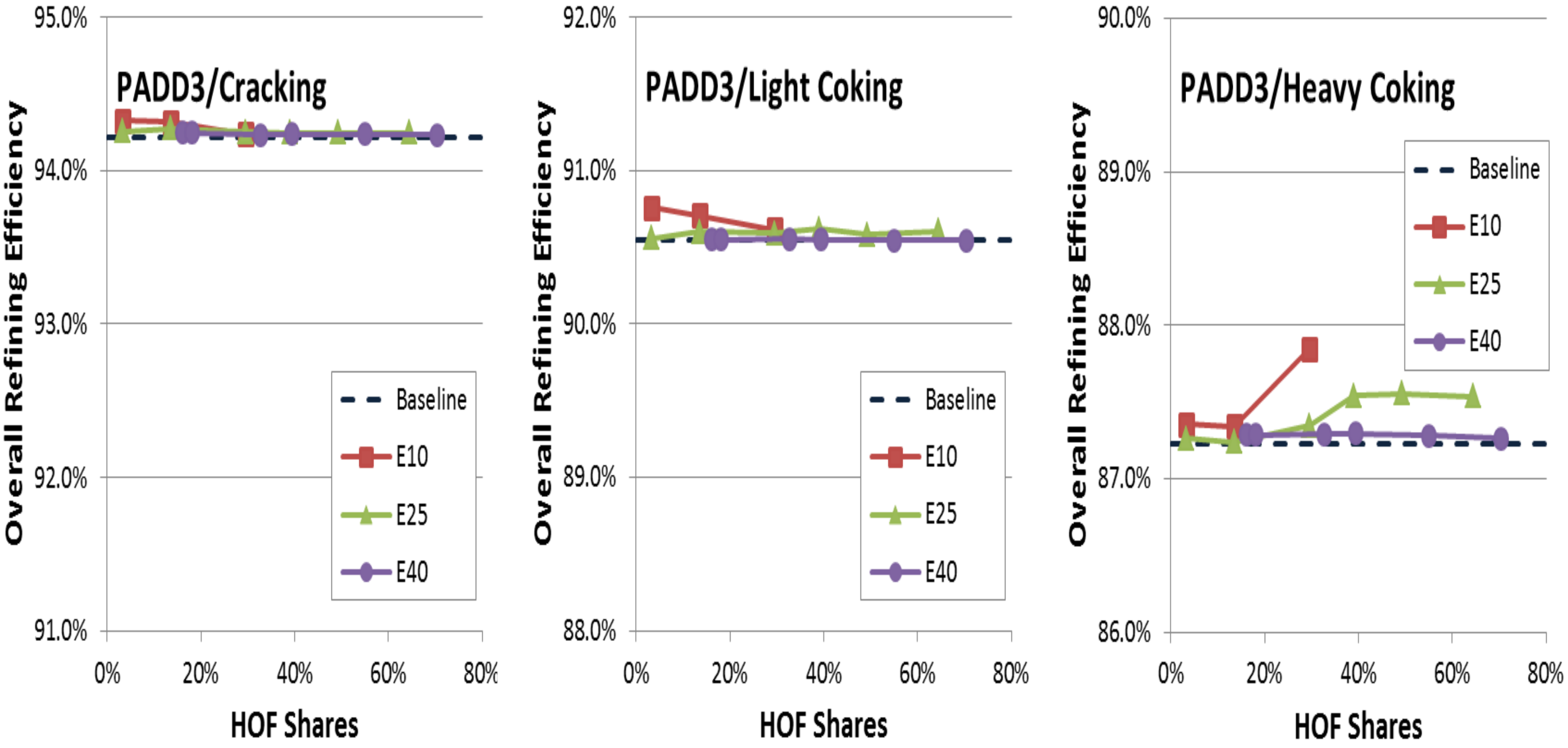
- Increasing ethanol blending level beyond E10 is more favorable for HOF RON and RVP

E10 HOF case operates the reformer at its maximum severity



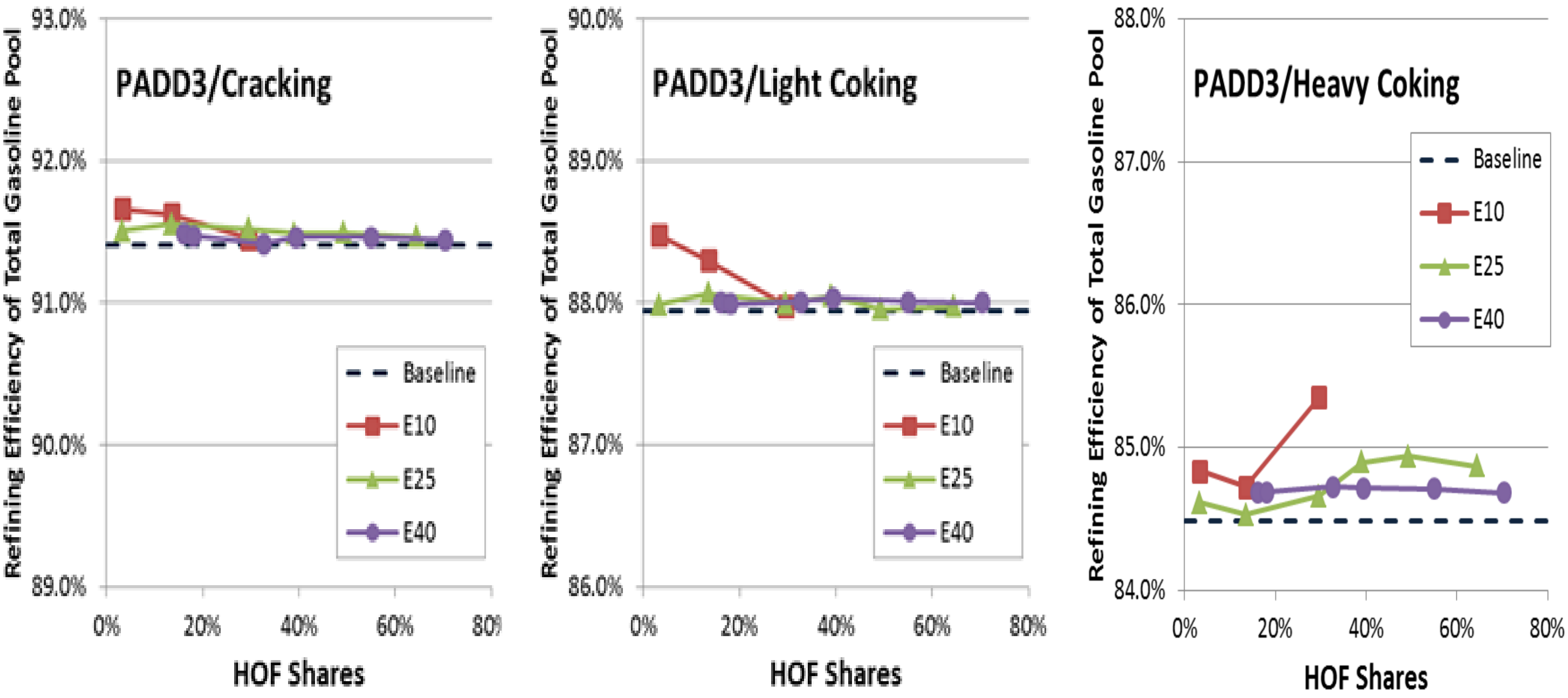
- Severity: RON of C5+ liquid product
- Higher severity → Low liquid yield
  → Negative impact on refinery margin

Overall refinery energy efficiency: configuration variation



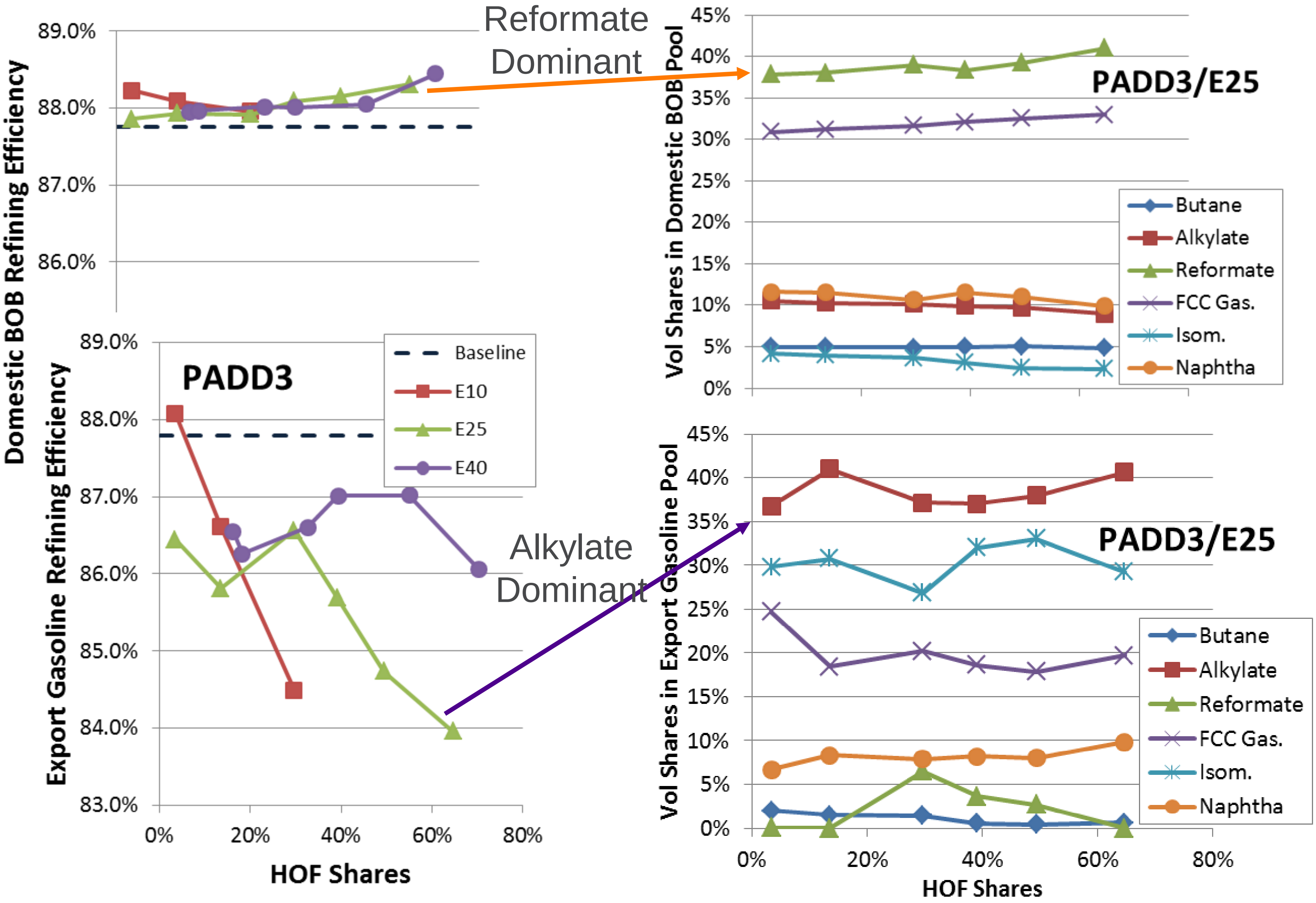
- Overall refinery efficiency drops as the complexity increases

Gasoline BOB refining energy efficiency: configuration variation



Argonne NATIONAL LABORATORY

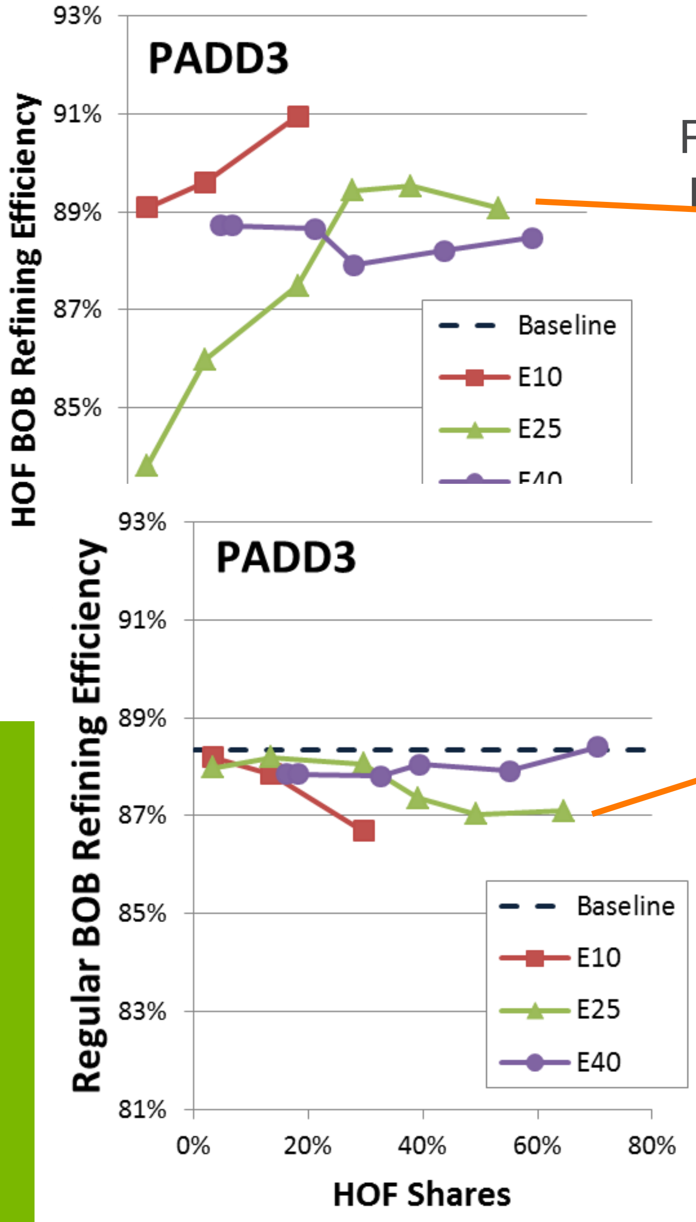
Domestic BOB vs. export gasoline: refining efficiency and gasoline pool composition



Reformate Dominant

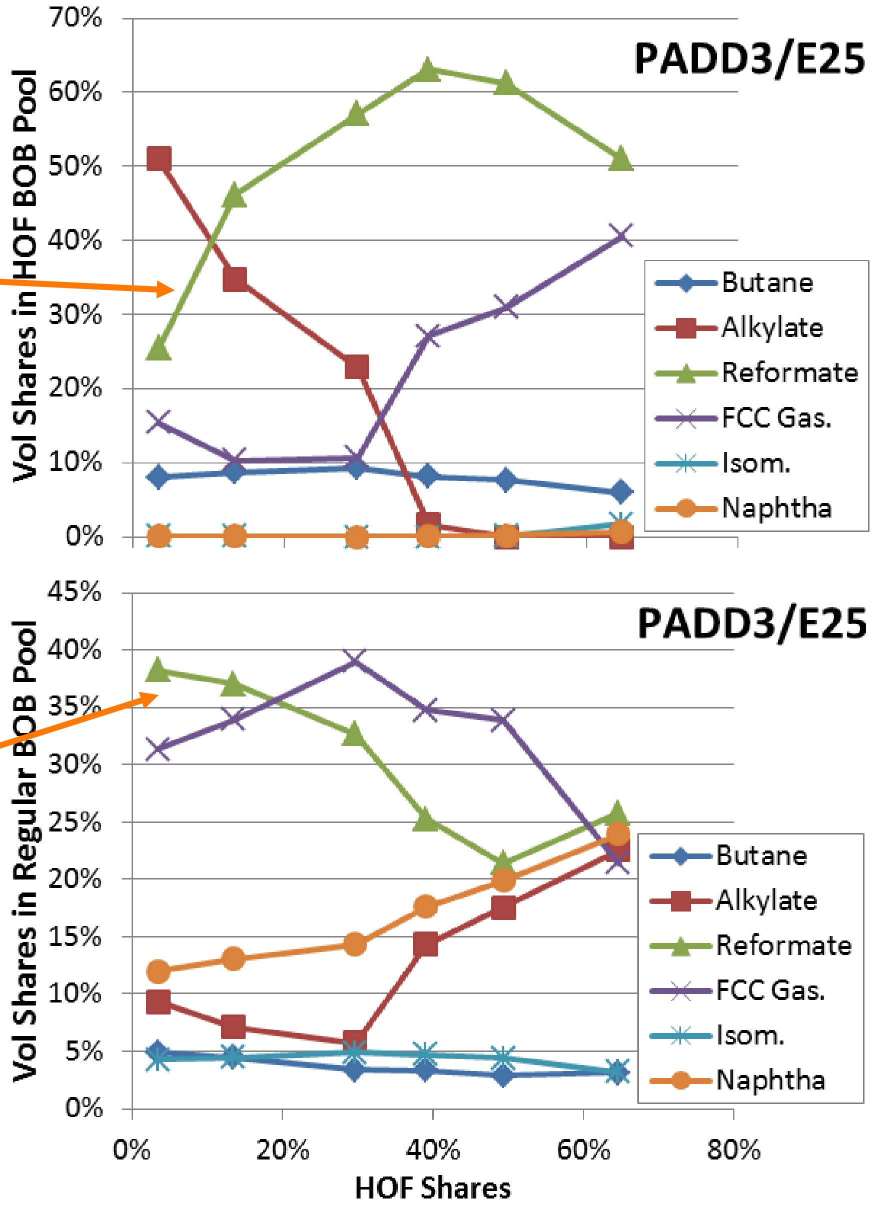
Alkylate Dominant

HOF vs. non-HOF BOB gasoline: refining Efficiency and gasoline pool composition

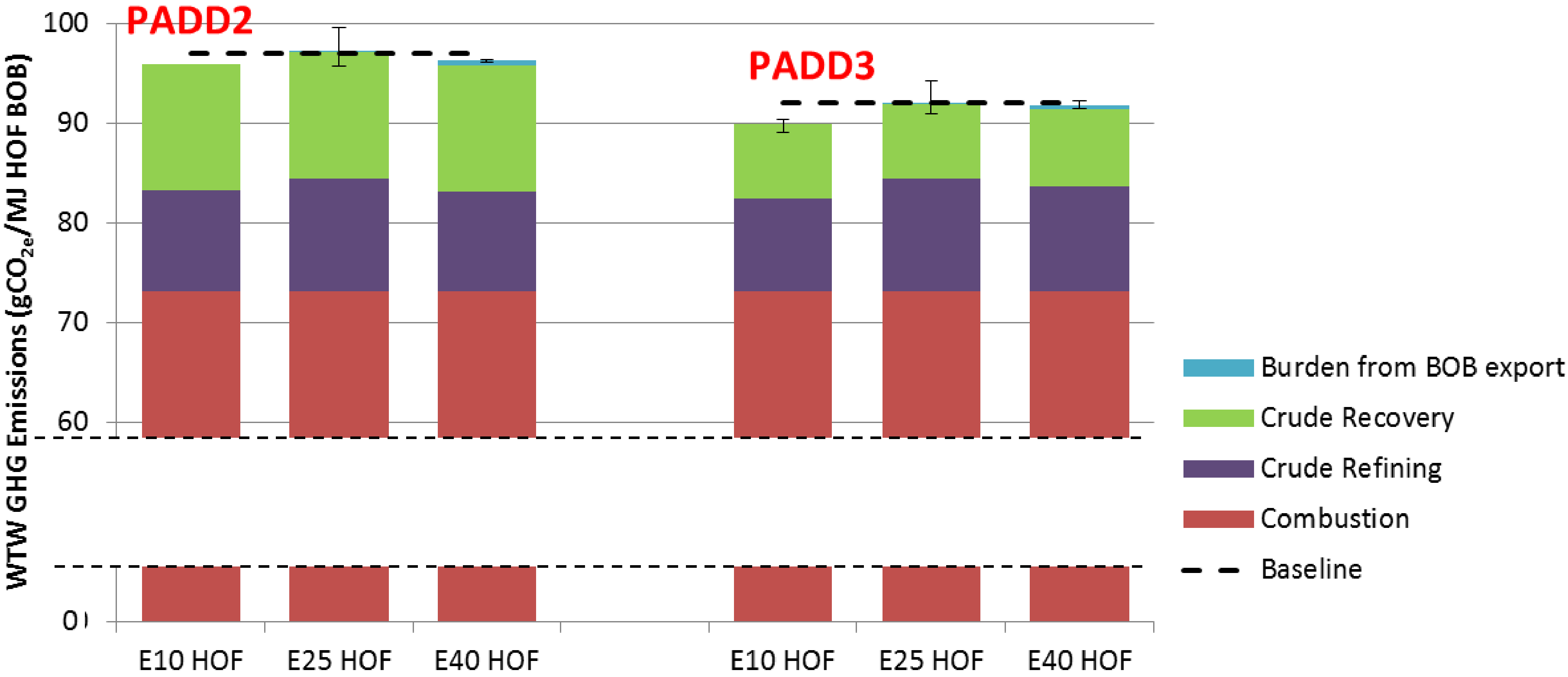


Reformate Dominant

Reformate Dominant



HOF BOB: GHG emission variation of HOF BOB component is small



- Larger WTW GHG emissions in PADD2 is due to a larger share of GHG-intensive oil sands
- Adjustment for the spill over is 0.2 gCO_2e/MJ of HOF on average (up to 0.8 gCO_2e)
- Baseline BOB is Business-As-Usual
  - Market shares of different gasoline types: 92% of regular E10 and 8% of premium E10

Please visit http://greet.es.anl.gov for:

- ***GREET models***
- ***GREET documents***
- ***LCA publications***
- ***GREET-based tools and calculators***