MODELING OF PETROLEUM REFINERIES FOR PRODUCING HIGH OCTANE FUELS AND THEIR WELL-TO-WHEELS ANALYSIS

Michael Wang, Jeongwoo Han, Amgad Elgowainy and Vince Divita
Argonne National Laboratory and Jacobs Consultancy

CRC Workshop on Life Cycle Analysis of Transportation Fuels
Argonne, IL
Oct. 27-28, 2015

Motivation for well-to-wheels (WTW) of high octane fuels (HOFs)

- Efficiency gains by vehicles fueled with HOFs have been suggested
- Ways of producing HOFs are being investigated
- Potential trade-offs between increased vehicle efficiencies and decreased HOF production efficiencies
- On the WTW basis, what are the net GHG effects?

Argonne Phase I HOF WTW report is available at:
https://greet.es.anl.gov/publication-high-octane-various-shares

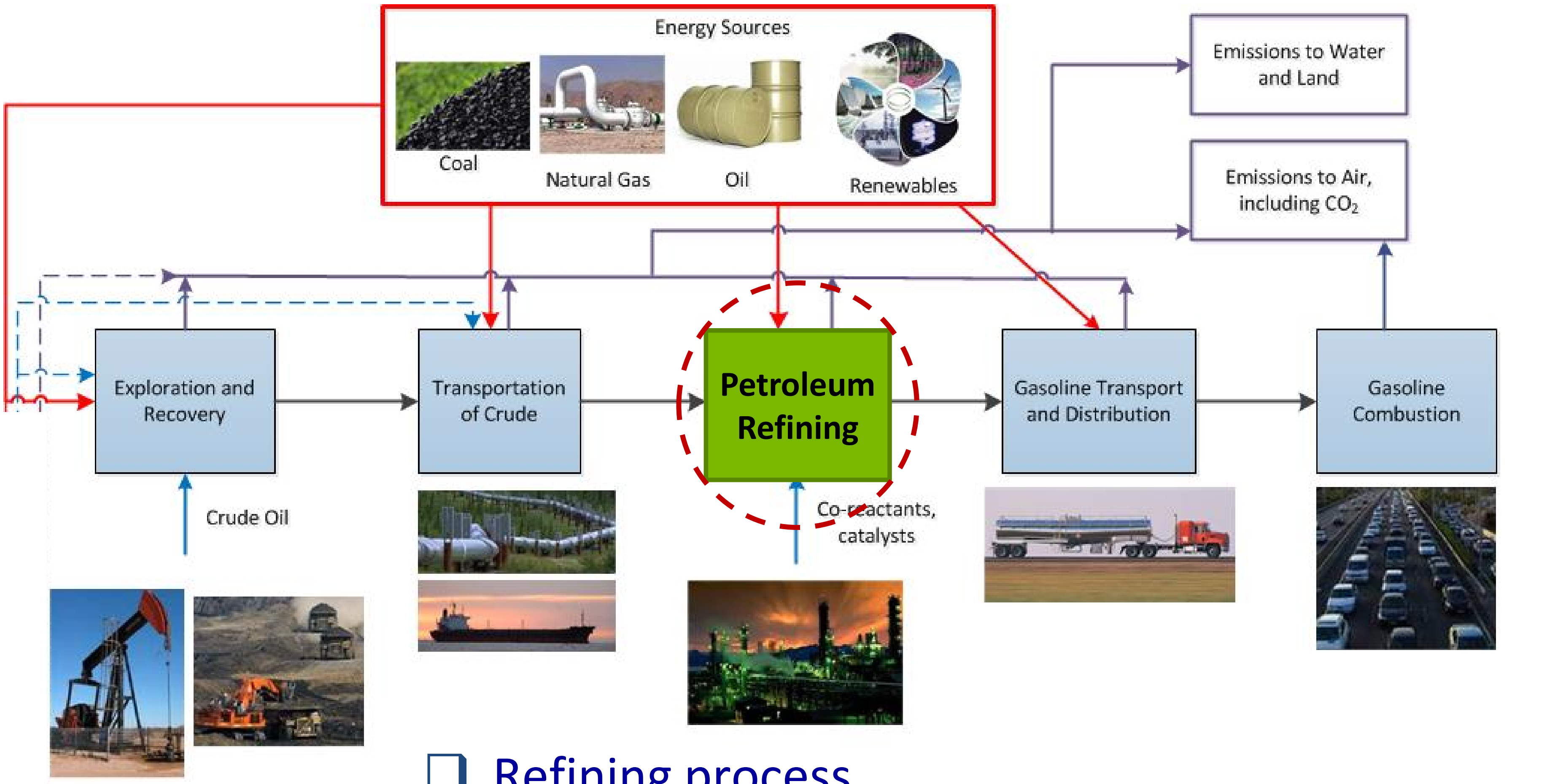
- Argonne's HOF WTW is part of the three-national lab efforts to address HOF potentials
  - ✓ Scope of the 3-lab study: understanding hurdles; proposing resolutions; quantifying potential benefits; and determining if additional R&D is warranted
  - ✓ Oak Ridge National lab: vehicle efficiency potentials and HOF market assessment
  - ✓ National Renewable lab: HOF fuel specs, distribution infrastructure needs, and market assessment
  - ✓ Argonne National Lab: WTW analysis; with Jacobs Consultancy on petroleum refinery LP modeling
- The 3-lab effort was supported by DOE
  - ✓ Bioenergy Technology Office sponsored the effort
  - ✓ Vehicle Technology Office and Energy Policy and System Analysis Office provided inputs

Argonne NATIONAL LABORATORY

ANL/ESD-15/10

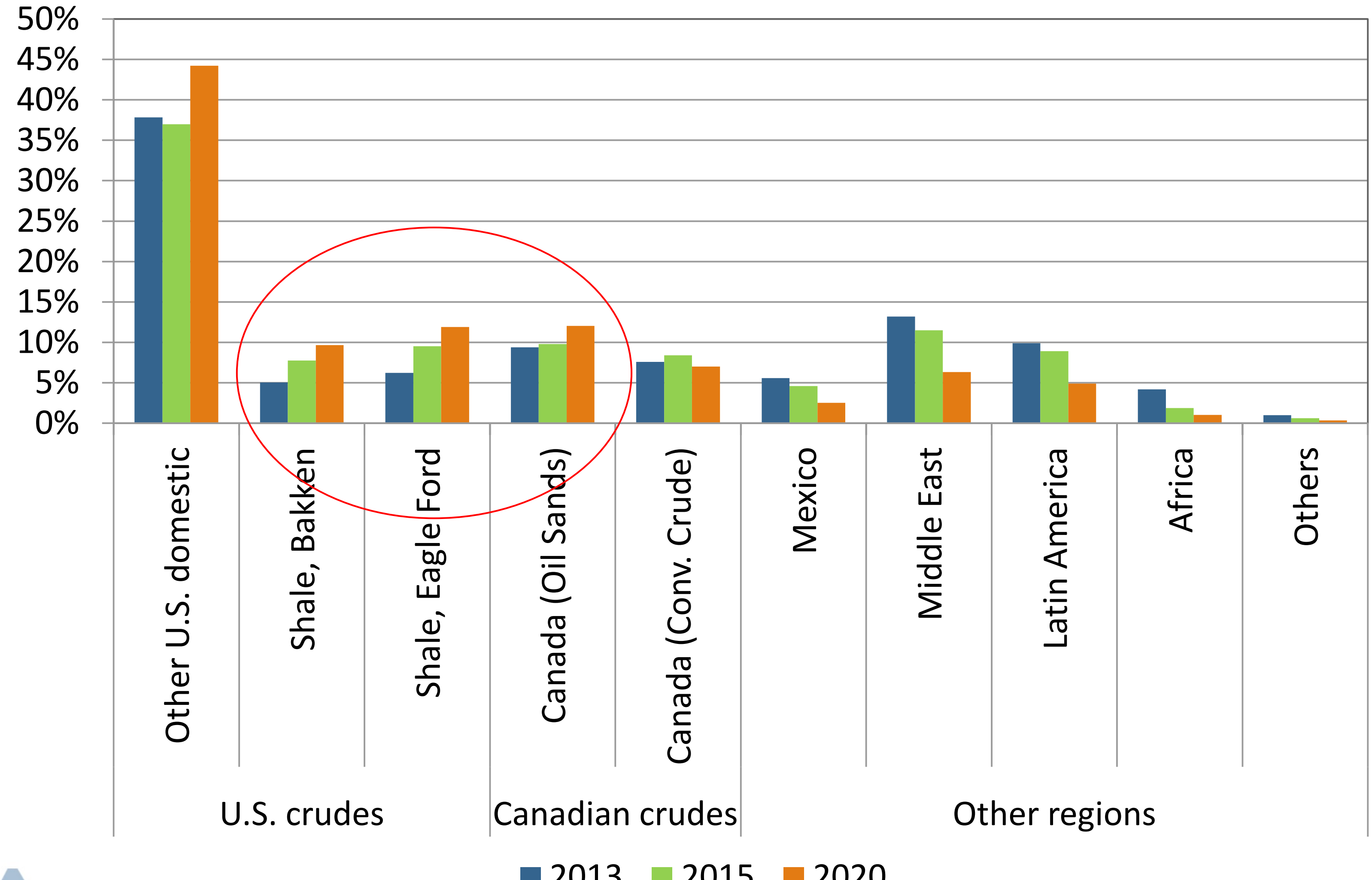
Well-to-Wheels Greenhouse Gas Emissions Analysis of High-Octane Fuels with Various Market Shares and Ethanol Blending Levels

WTW analysis of petroleum fuels pathways

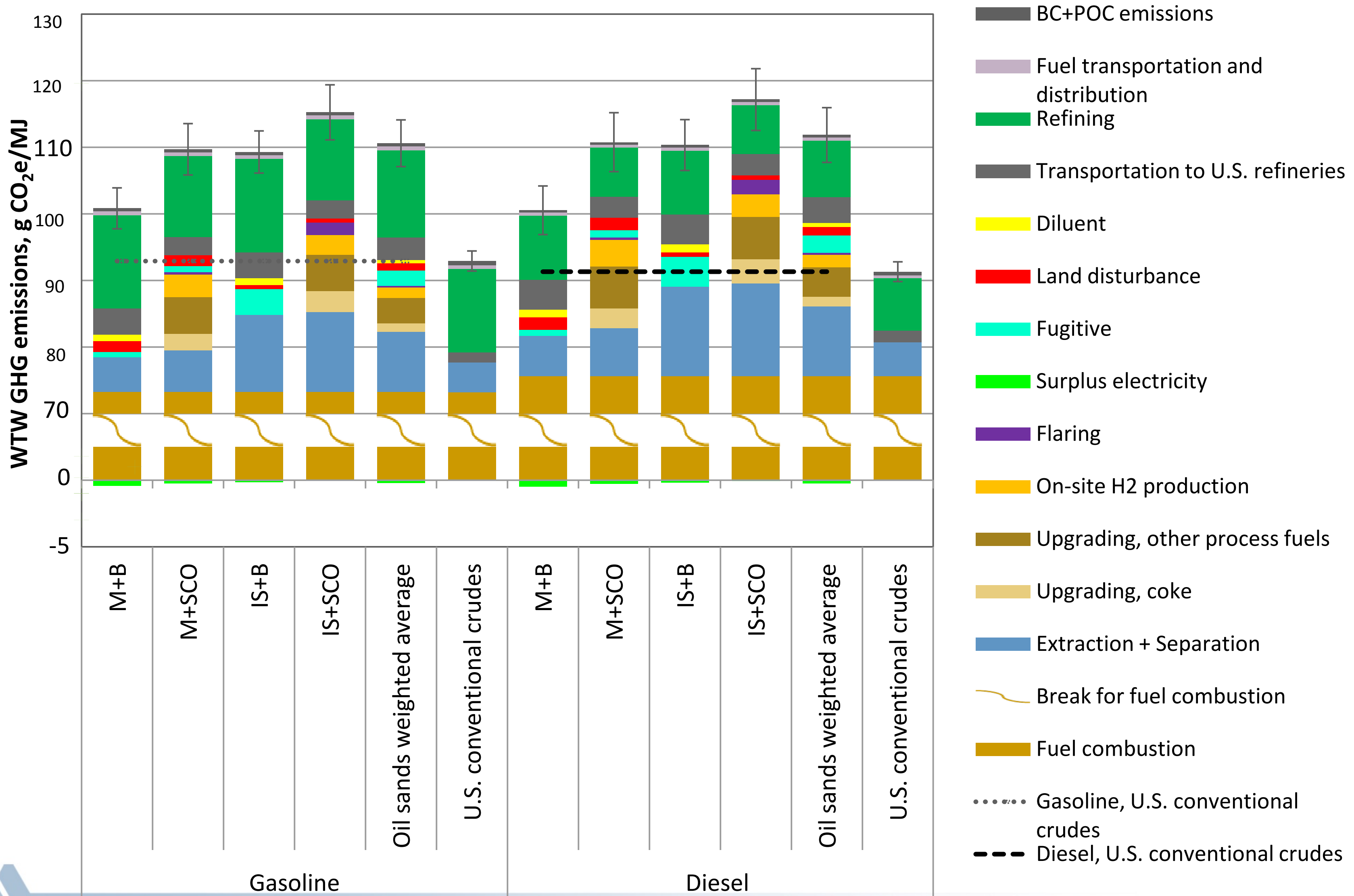


- ❑ Refining process
  - ✓ Second-largest GHG emissions source in fuel cycle
  - ✓ Complex system with multiple co-products
  - ✓ Key process for assessing the impact of producing HOF

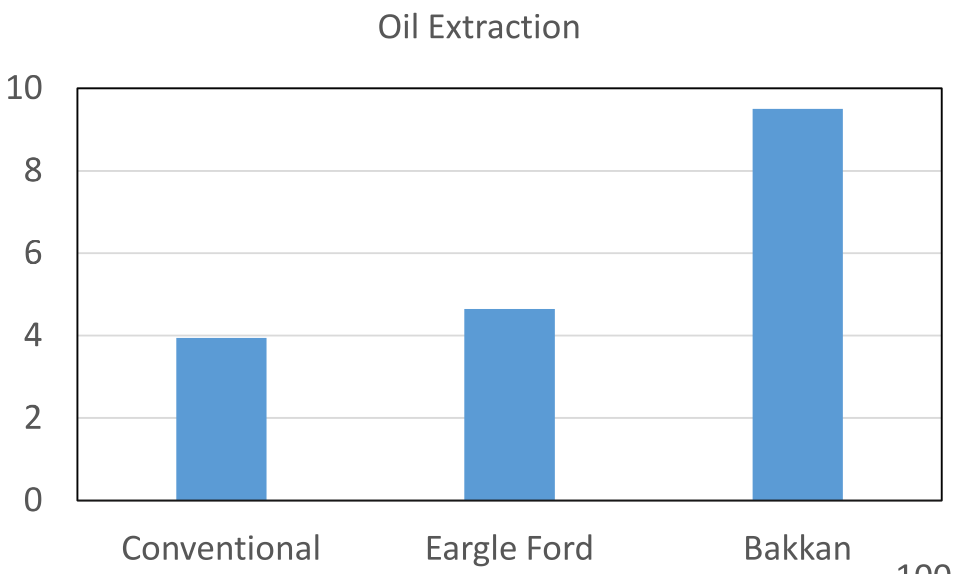
Canadian oil sands and shale oil shares are increasing in the U.S. crude oil mix



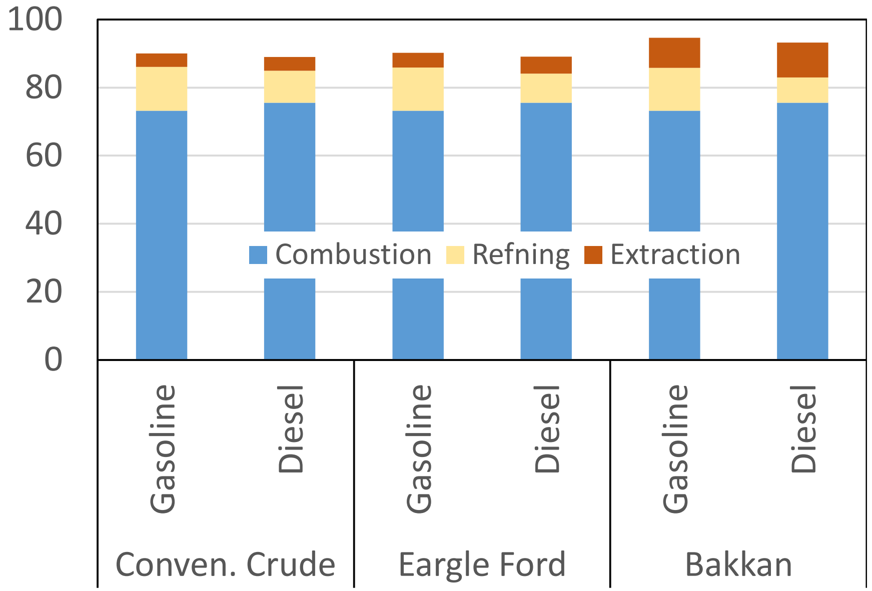
Oil sands-derived gasoline and diesel have about 20% higher GHG intensities



WTW GHG emissions of conventional oil vs. shale oil: g CO2e/MJ

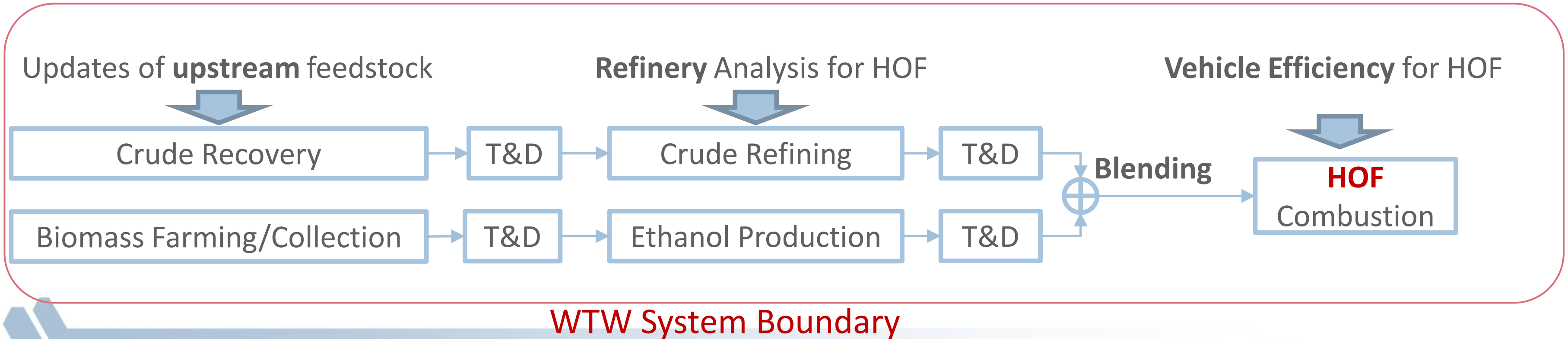


Sources:
Eagle Ford: Yeh et al. 2015
Bakkan: Brandt et al. 2015

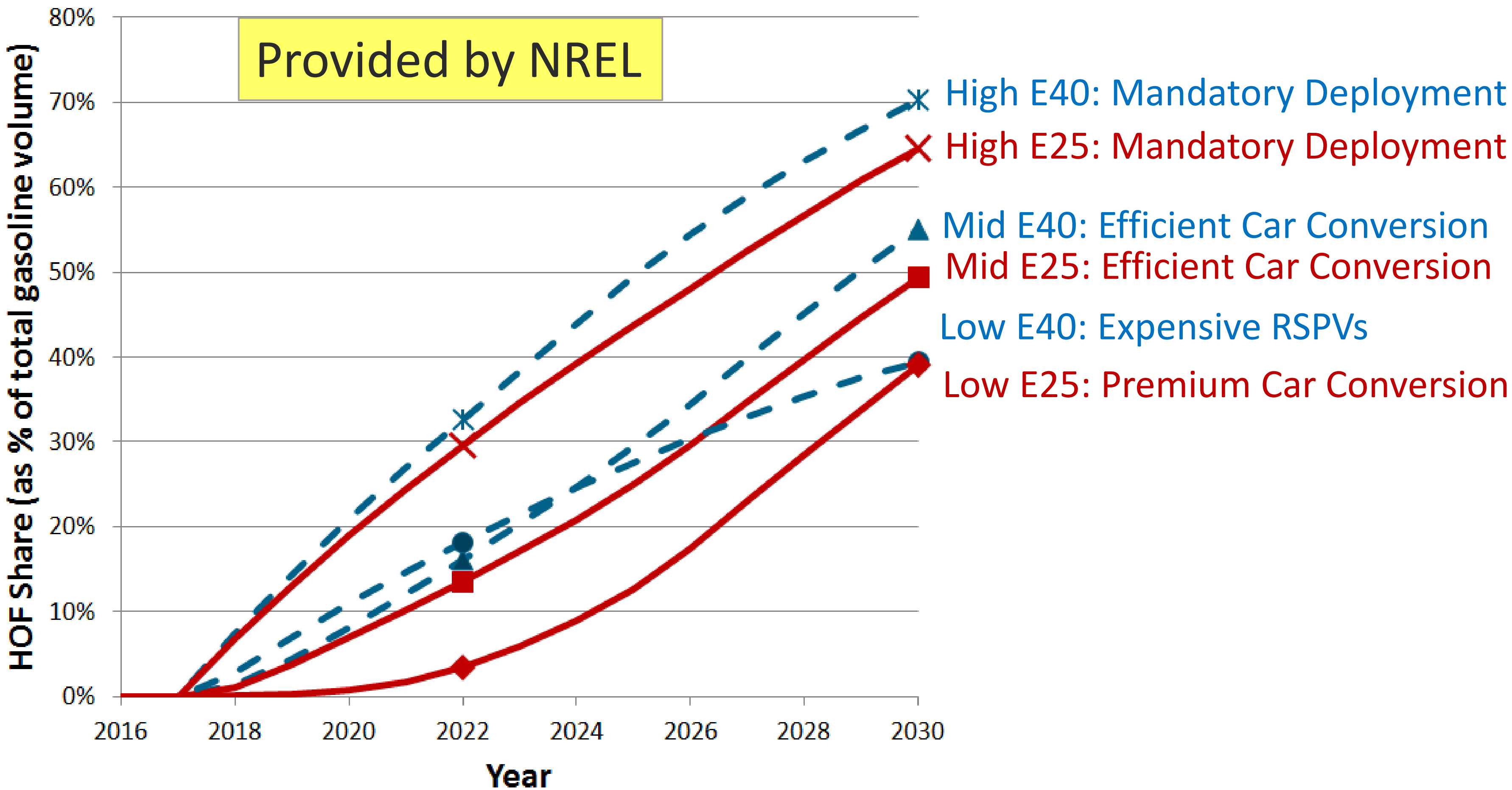


HOF WTW technical approach

- New engine/vehicle technologies are to introduce to benefit from high octane
- Ethanol from corn and cellulosic biomass is simulated with the GREET framework
- HOF is produced at refineries with current gasoline fuel (E10) and increased ethanol blending levels (E25 and E40)
- Petroleum refinery LP modeling to address energy use and GHG emissions of HOF (RON 100) production
  - Baseline fuel (E10, RON 92)
  - Research Octane Number (RON)
  - Reid Vapor Pressure (RVP)
  - Refinery configurations
  - Inputs of different crude types
  - Ethanol blending for HOF RON
- Crude types
  - US conventional crude
  - Canadian oil sands
  - Shale oil (not included in Phase 1 simulations)



HOF market share is a key WTW parameter for LP modeling

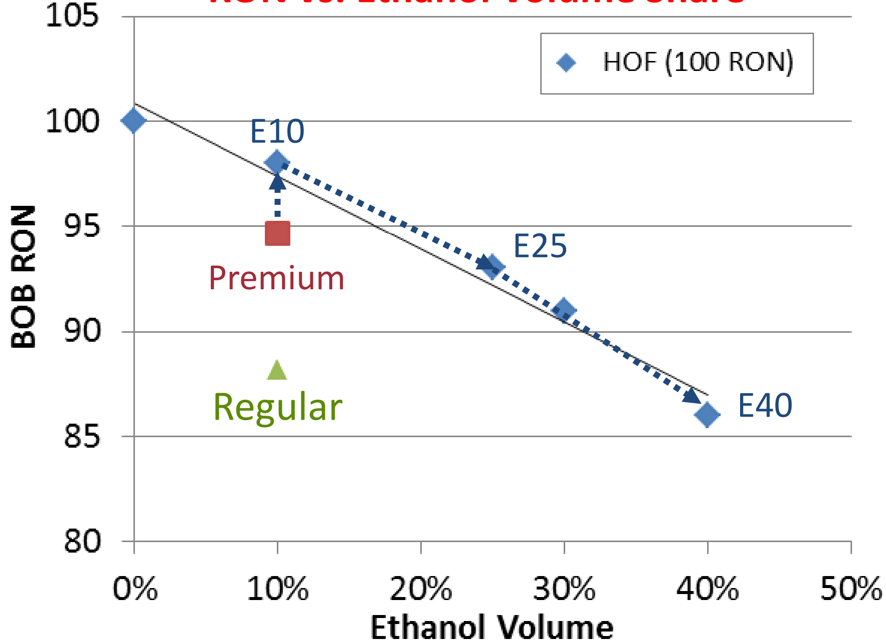


- Years **2022** and **2030** are selected for refinery LP modeling
  - ✓ Covers the entire range of HOF market shares

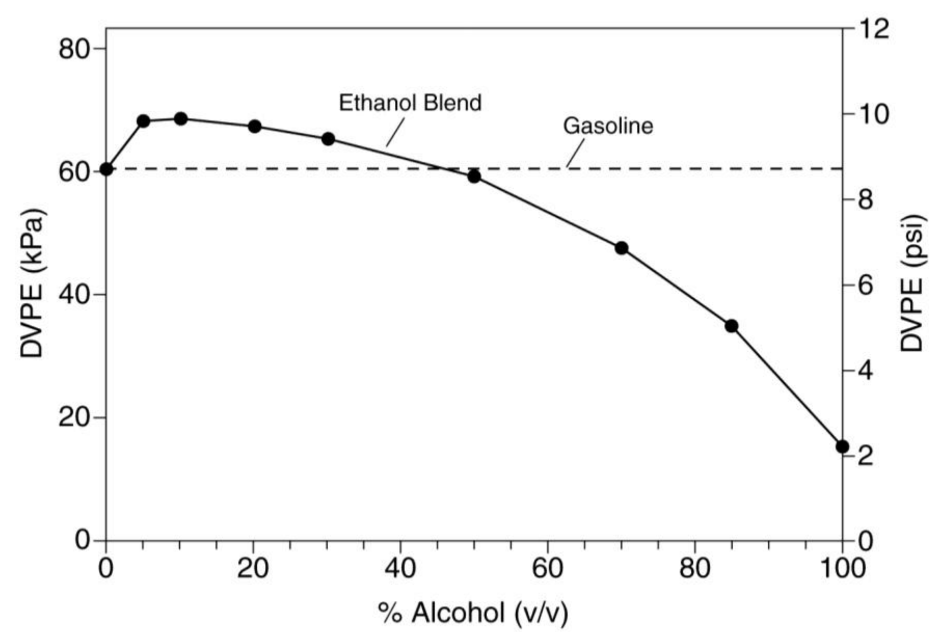
Research Octane Number (RON) and Reid Vapor Pressure (RVP) are key fuel specifications

	Regular gasoline (E10)	Premium gasoline	HOF E10	HOF E25	HOF E40
Fuel RON	91	95.6	100	100	100
BOB RON	88 - 89	93 - 94	98	93	86
CG Summer RVP (psi)	9	9	9	**8**	**8**
CBOB Summer RVP (psi)	7.8	7.8	7.8	7.0	6.8
RFG Summer RVP (psi)	7	7	**9**	7	7
RBOB Summer RVP (psi)	5.6	5.6	**7.8**	5.7	5.1

RON vs. Ethanol Volume Share



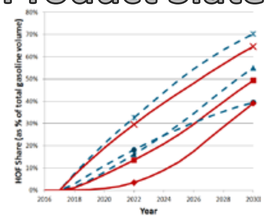
RVP vs. Ethanol Volume Share

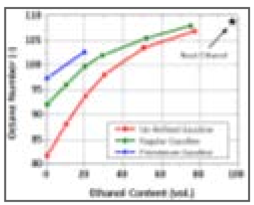


Detailed refinery LP modeling needed for reliable WTW

Crude Slate

Product Slate

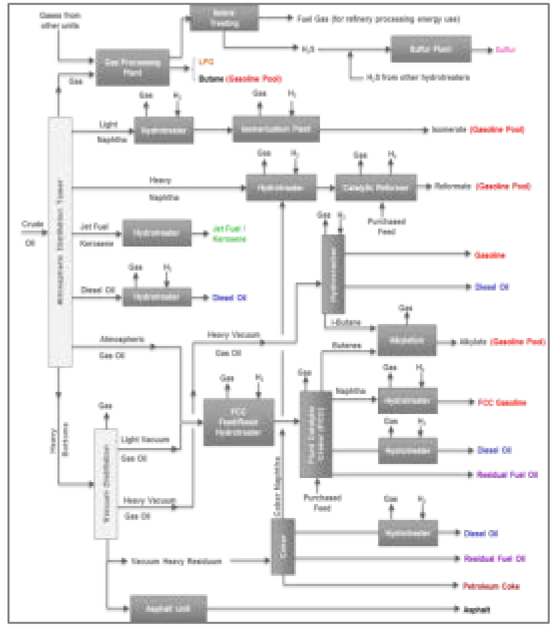




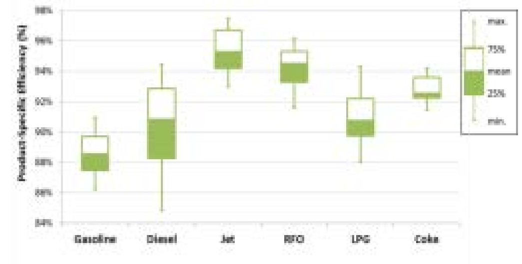
Fuel Specifications
(RON, RVP)

Economic
factors

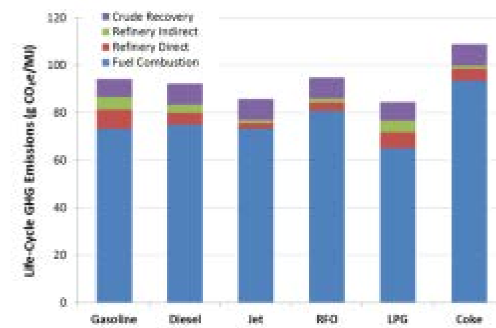
Refinery LP Modeling



Refining Efficiency



Life-Cycle Analysis

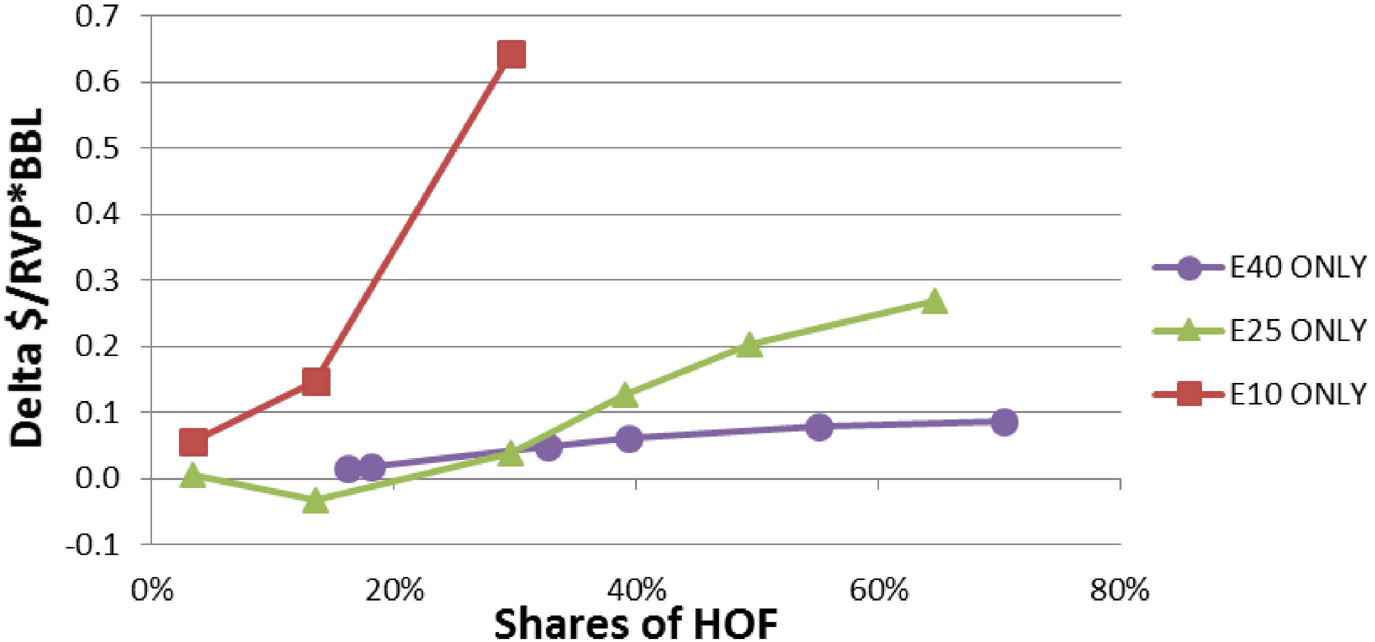


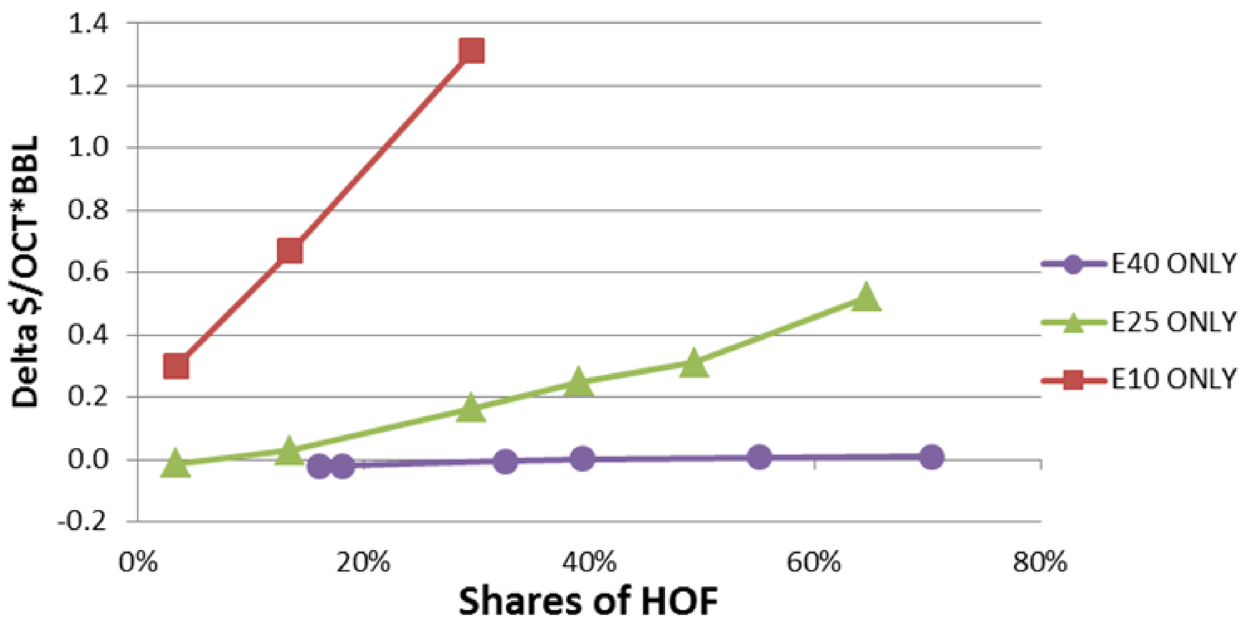
- ❑ Reliable modeling of complex refinery industry
- ❑ Detailed modeling results of refining process units, intermediate products flow rates, utility consumptions, etc.
  - ✓ To evaluate the energy and emissions burden of individual refinery products

Other key assumptions for refinery LP modeling

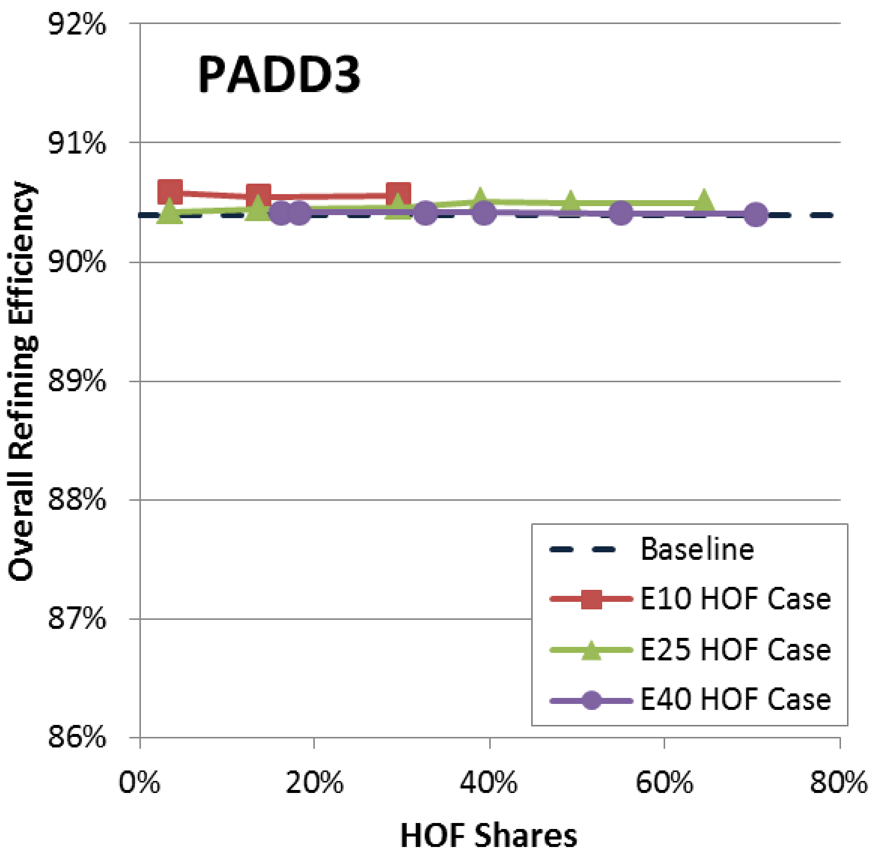
- Refinery LP models based on **actual refinery configurations** reported by Oil and Gas Journal
  - ✓ Two regions (**PADD3** and **PADD2**)
  - ✓ Three refinery configuration types: cracking, light coking and heavy coking
  - ✓ Each configuration meets the 100 RON HOF shares separately
- **No new capital investment** is assumed
- **Crude slates** for each region are from **AEO projections to 2020**
- The **price** of HOF and non-HOF is set to **conventional gasoline price per volume** (Fuel Parity → MPG gain assumed to compensate for decreased volumetric energy density)
- **Gasoline Export** is allowed after the US gasoline demands are met
  - ✓ Discount for exported gasoline: 6 and 10 cent per gallon for PADD3 and PADD2, respectively

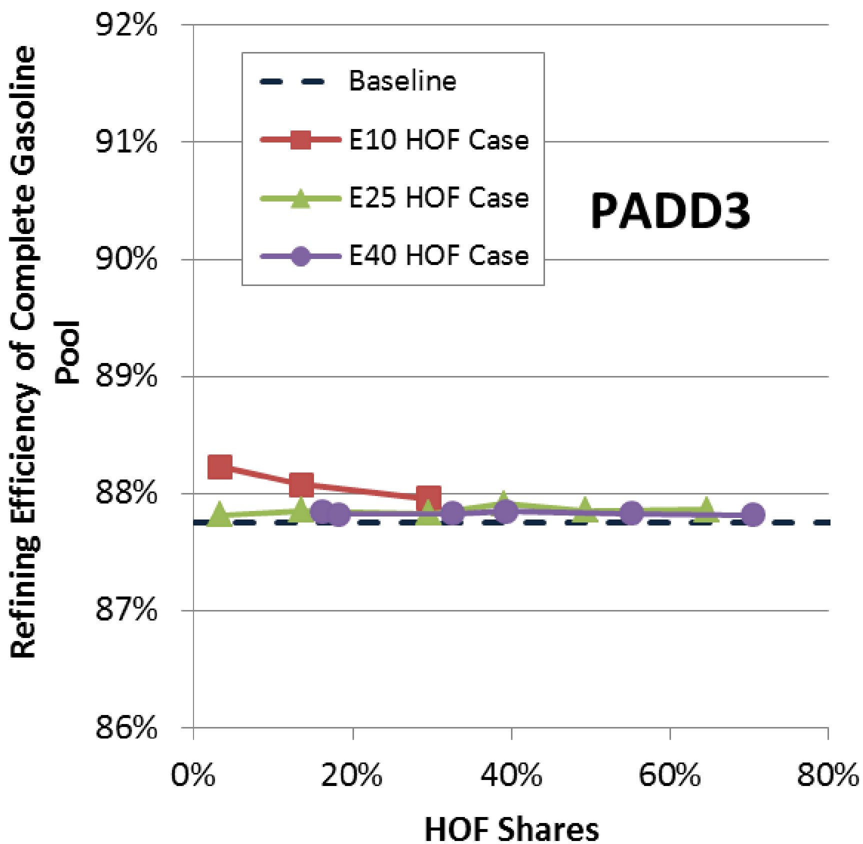
Marginal RVP and RON cost relative to the baseline case





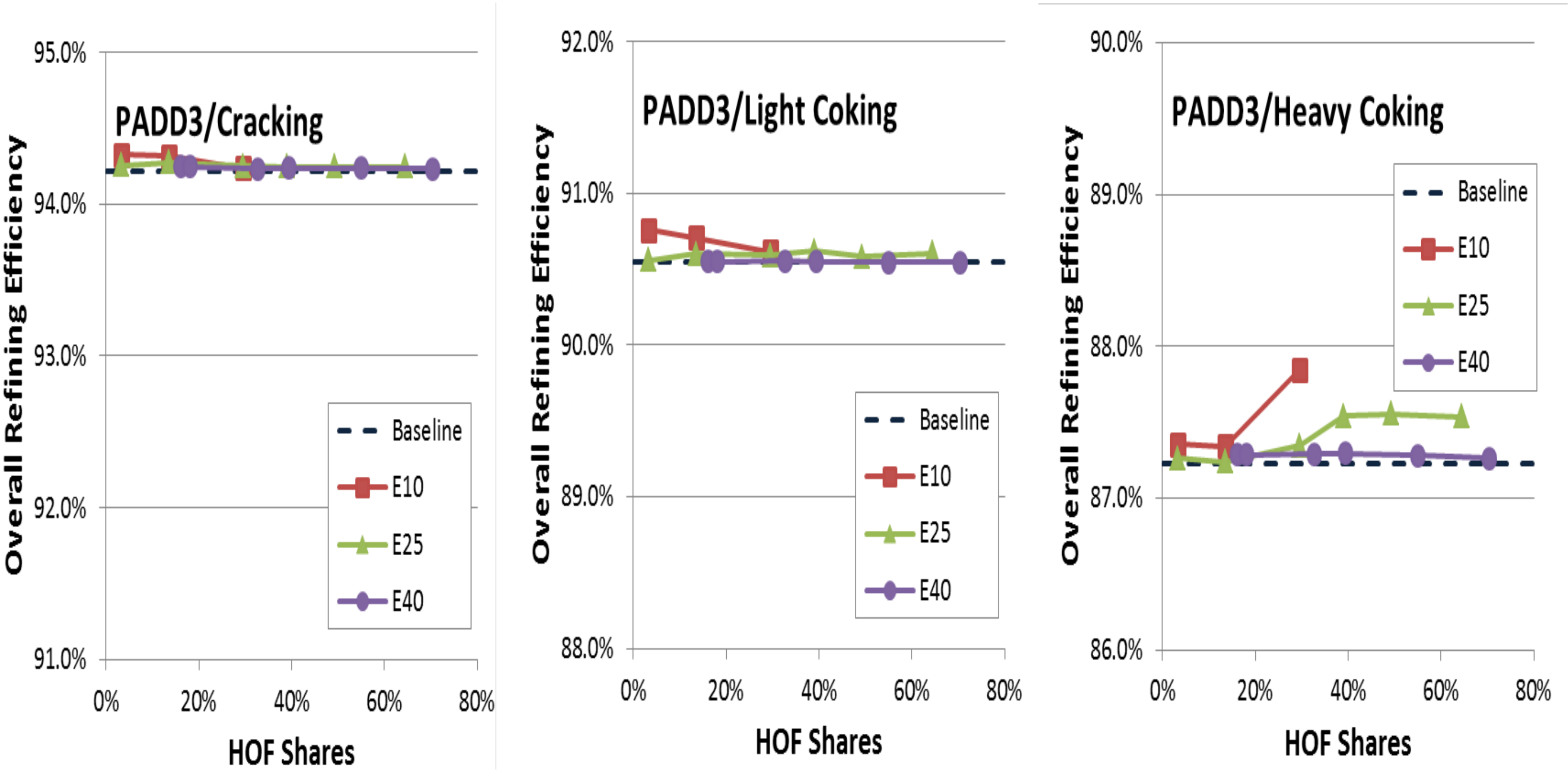
Small change in overall refinery and gasoline BOB energy efficiencies with ethanol blending level and HOF share





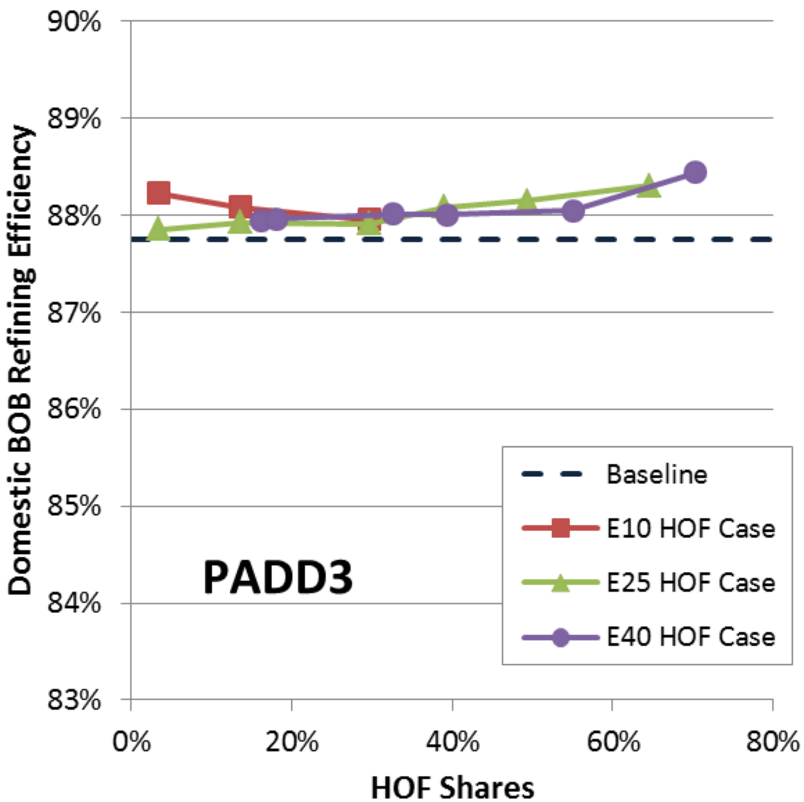
- BOB + Ethanol = Finished Gasoline
- E10 HOF is feasible only up to ~25% of gasoline market share
  - ✓ A result of **no new capital investment assumption**
- PADD2 shows similar trends

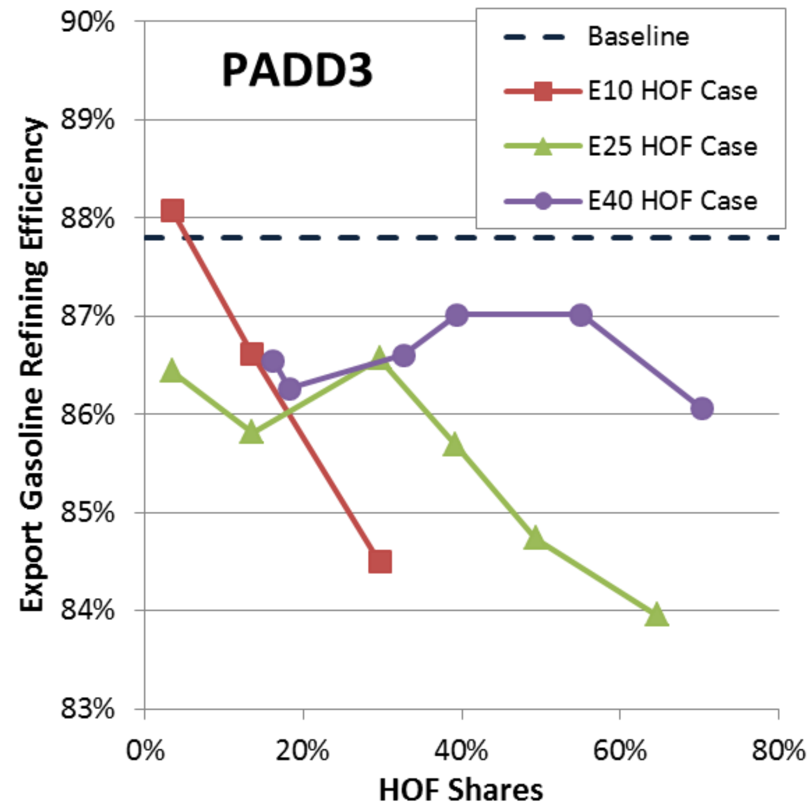
Overall refinery energy efficiency: configuration variation



- Overall refinery efficiency drops as the refinery complexity increases
- Capacity share: cracking 20%; light coking 50%; heavy coking 30%

Refining efficiencies of domestic BOB and exported gasoline vary

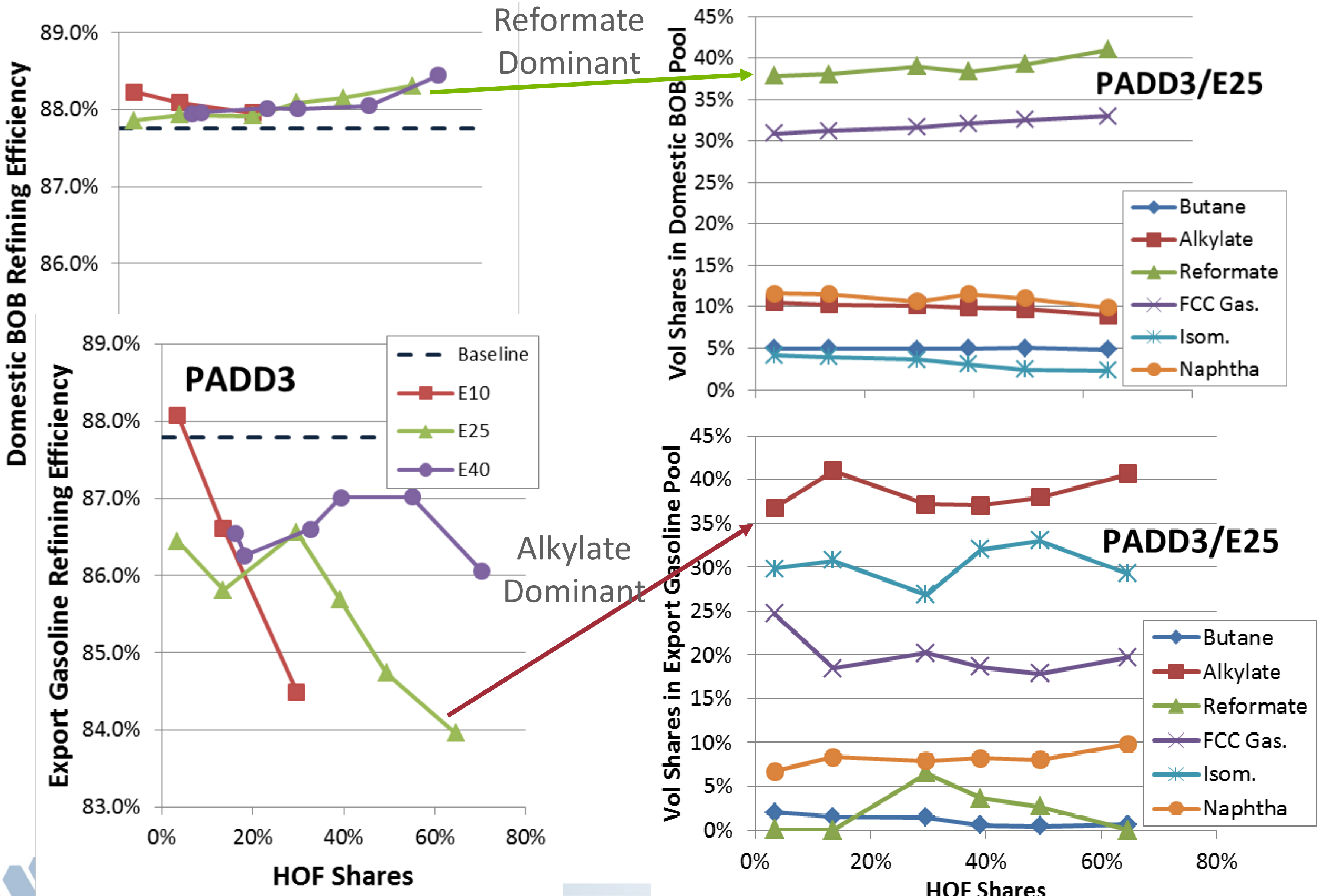




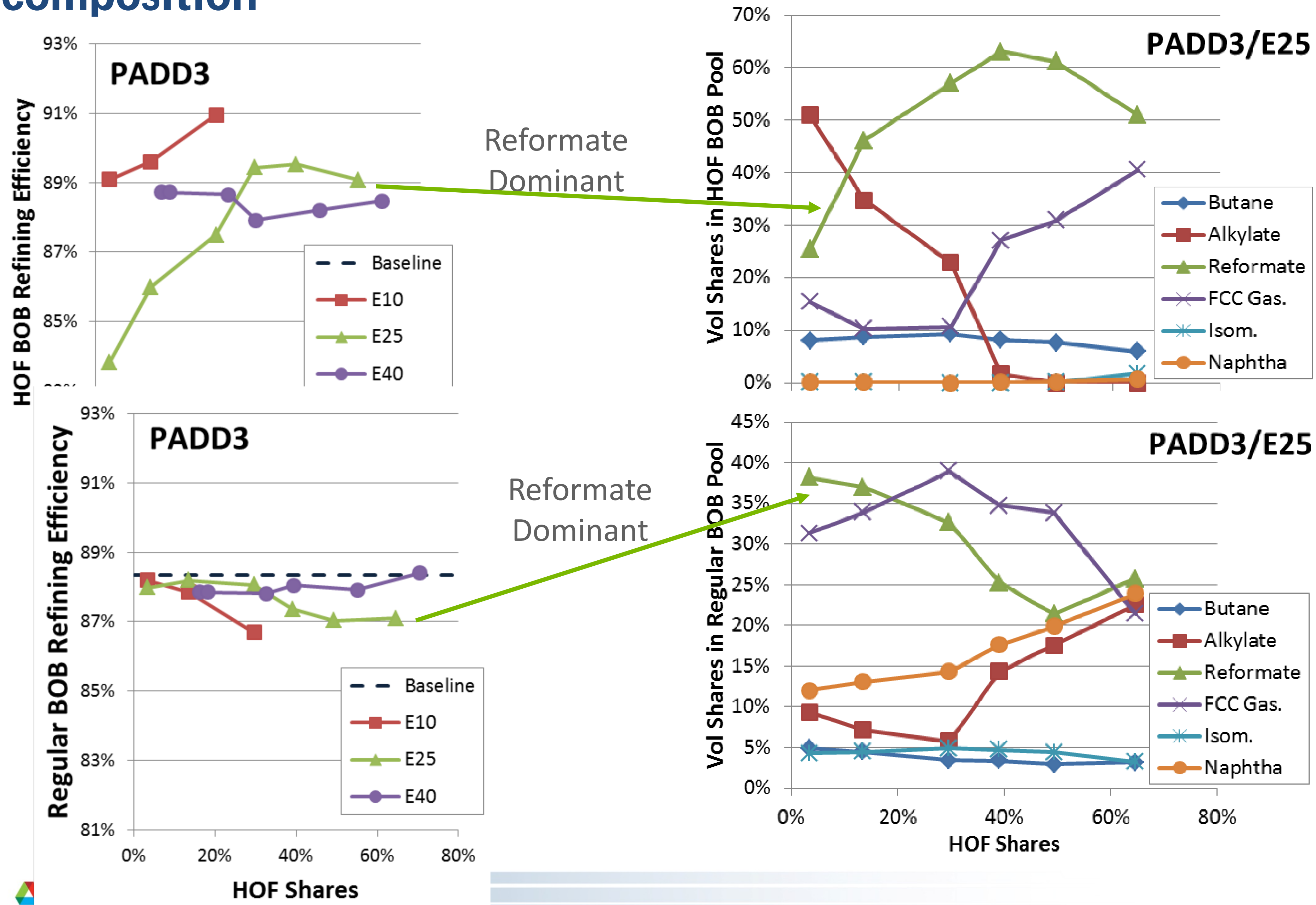
Possible spill over of energy penalty from domestic BOB to exported gasoline pool

- Up to 4% drops in exported gasoline refining efficiency from the baseline (non-HOF) case
- Up to 2.5 g CO2e/MJ increases in exported gasoline's GHG emissions from the baseline
  - ✓ But impact on HOF is small (<1 gCO_2e/MJ HOF)
- Domestic BOB share >90%; exported gasoline share <8-9%

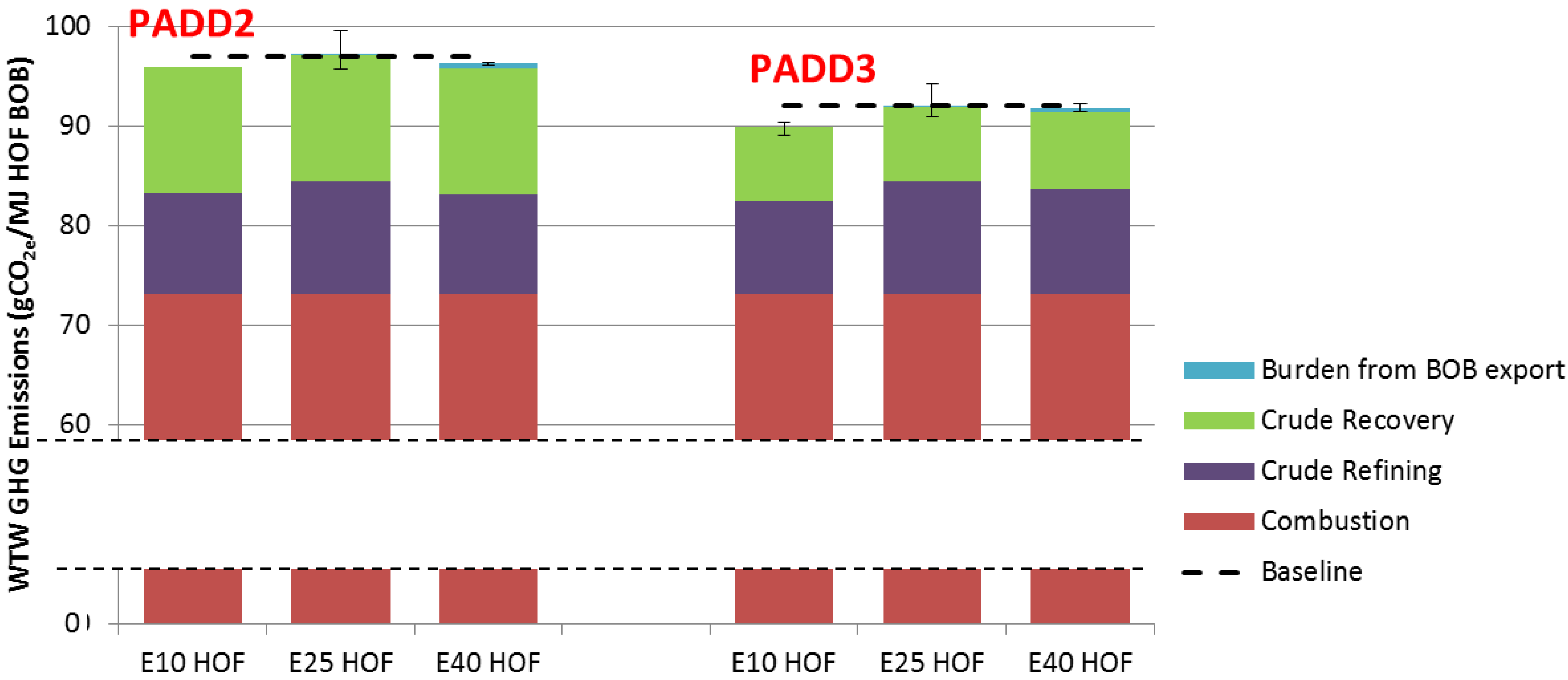
Domestic BOB vs. exported gasoline: refining efficiency and gasoline pool composition



HOF vs. non-HOF BOB: refining efficiency and BOB pool composition

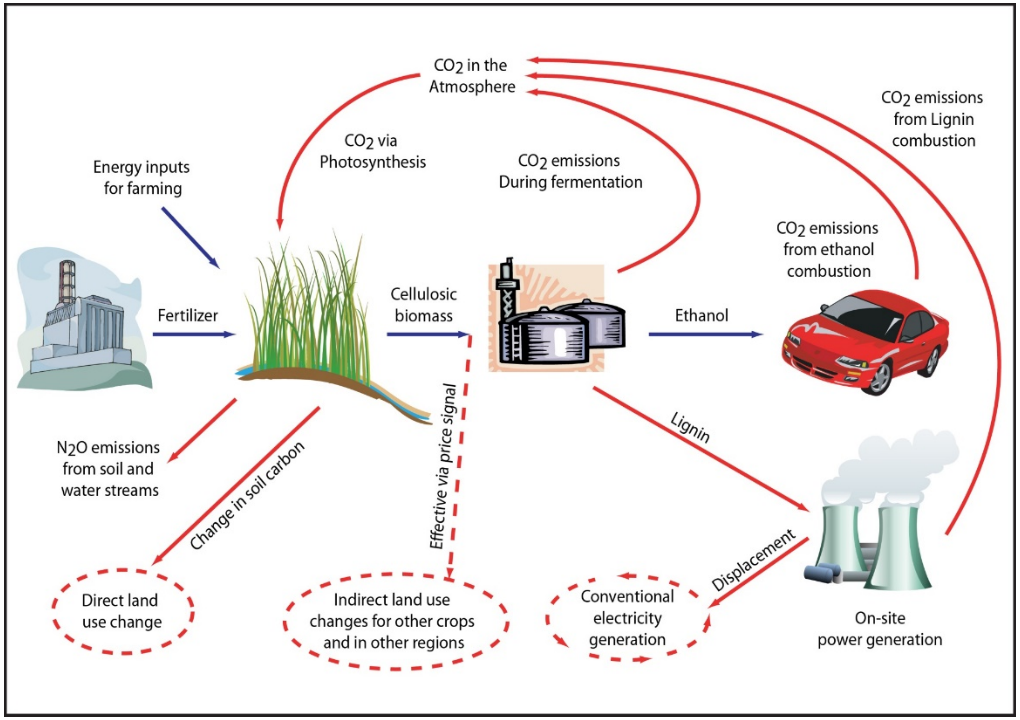


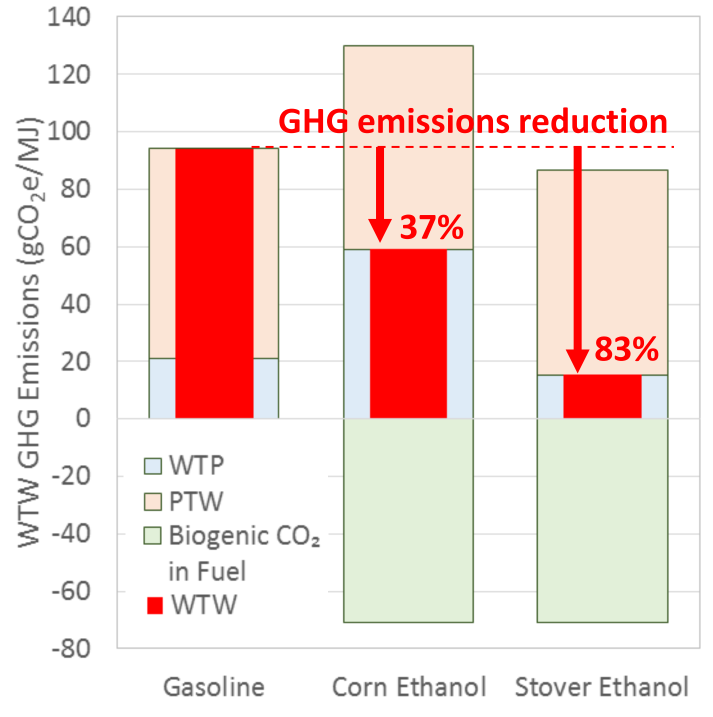
HOF BOB: GHG emission variation of HOF BOB component is small



- Larger WTW GHG emissions in PADD2 is due to a larger share of GHG-intensive oil sands
- Baseline BOB is Business-As-Usual
  - Market shares of different gasoline types: 92% of regular E10 and 8% of premium E10
- E10 HOF BOB is benefited from 1 psi waiver; E40 HOF BOB is benefited from E40 reduction in refinery severity

WTW analysis of ethanol from corn and corn stover



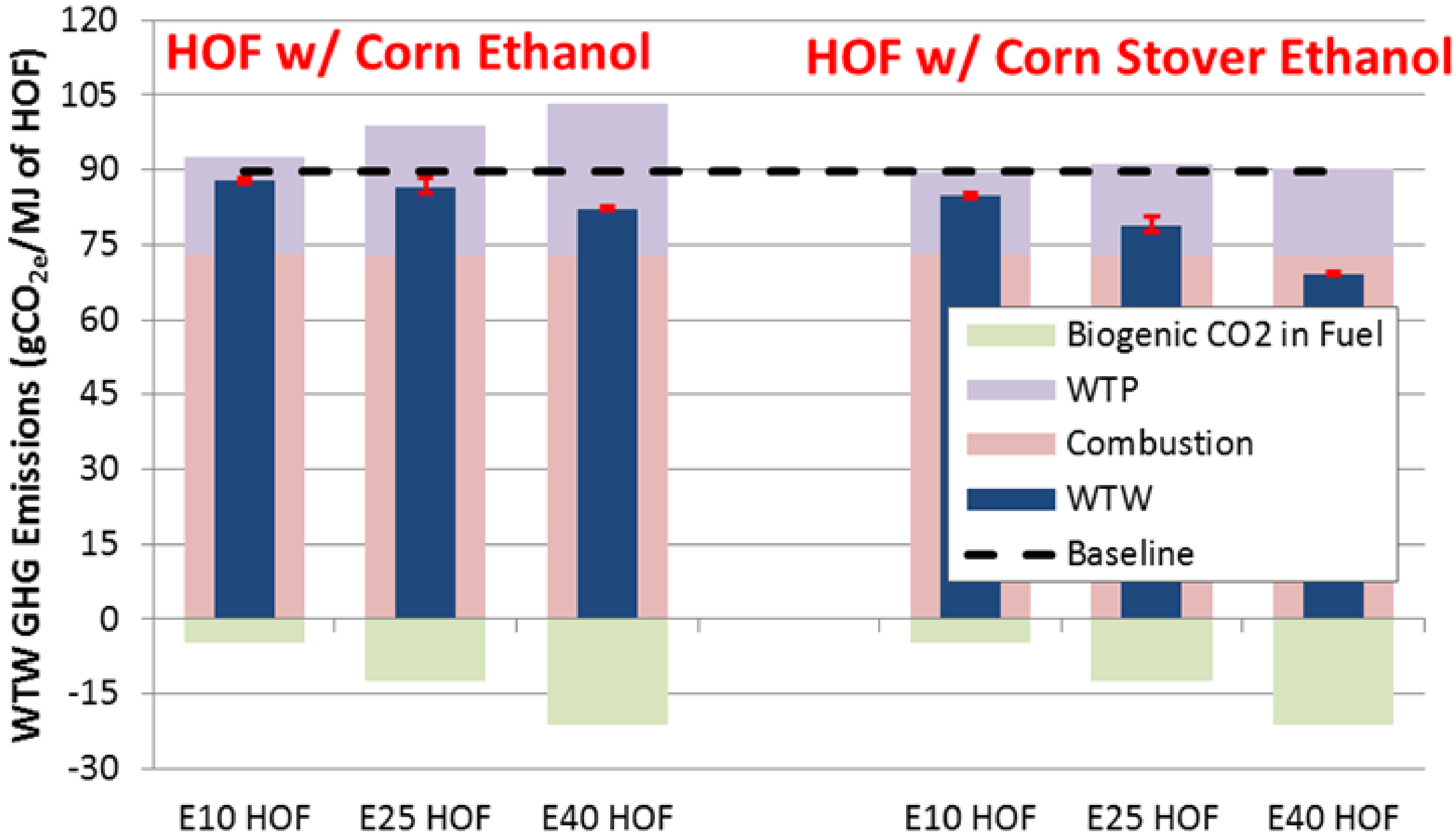


Key Parameters for 2022-2030

	Corn	Stover
Farming energy use	8,700 Btu/bushel	190,000 Btu/dry ton
Nitrogen fertilizer	380 g/bushel	7,000 g/dry ton
Ethanol yield	2.93 gal/bushel	90 gal/dry ton
Ethanol plant fossil energy use	28,000 Btu/gal ethanol	N/A
Coproduct yield	5.39 dry lb DGS/gal ethanol[1] 0.56 lb corn oil/bushel corn[1]	2.3 kWh electricity/gal ethanol
LUC GHG emissions	8 g CO2e/MJ ethanol	-0.7 g CO2e/gal ethanol

[1] Dry mill with corn oil extraction case (73% share)

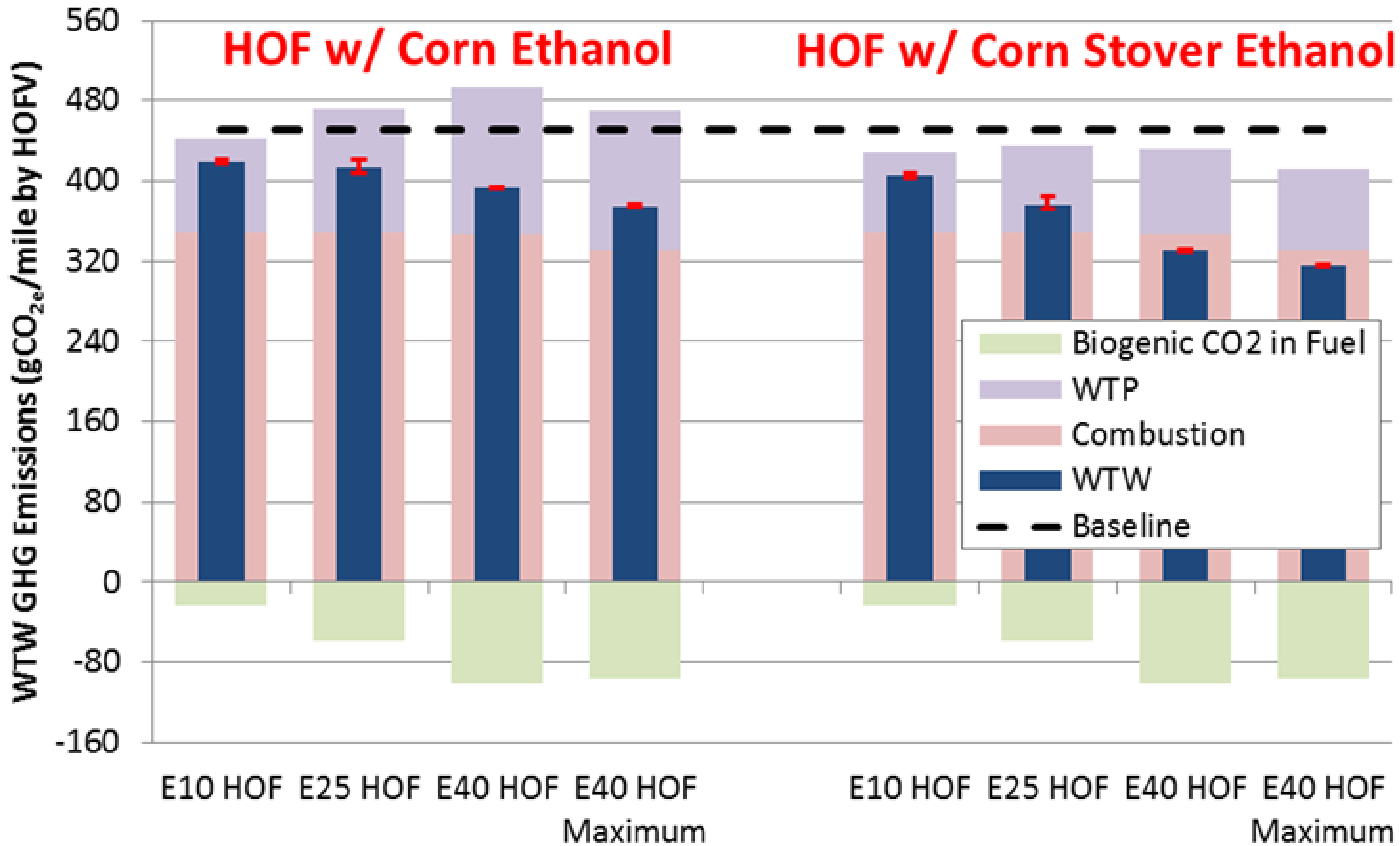
Finished HOF: higher ethanol blending level contributes to lower WTW GHG emissions of HOF (per MJ result, PADD3)



Potential vehicle efficiency gains of HOF

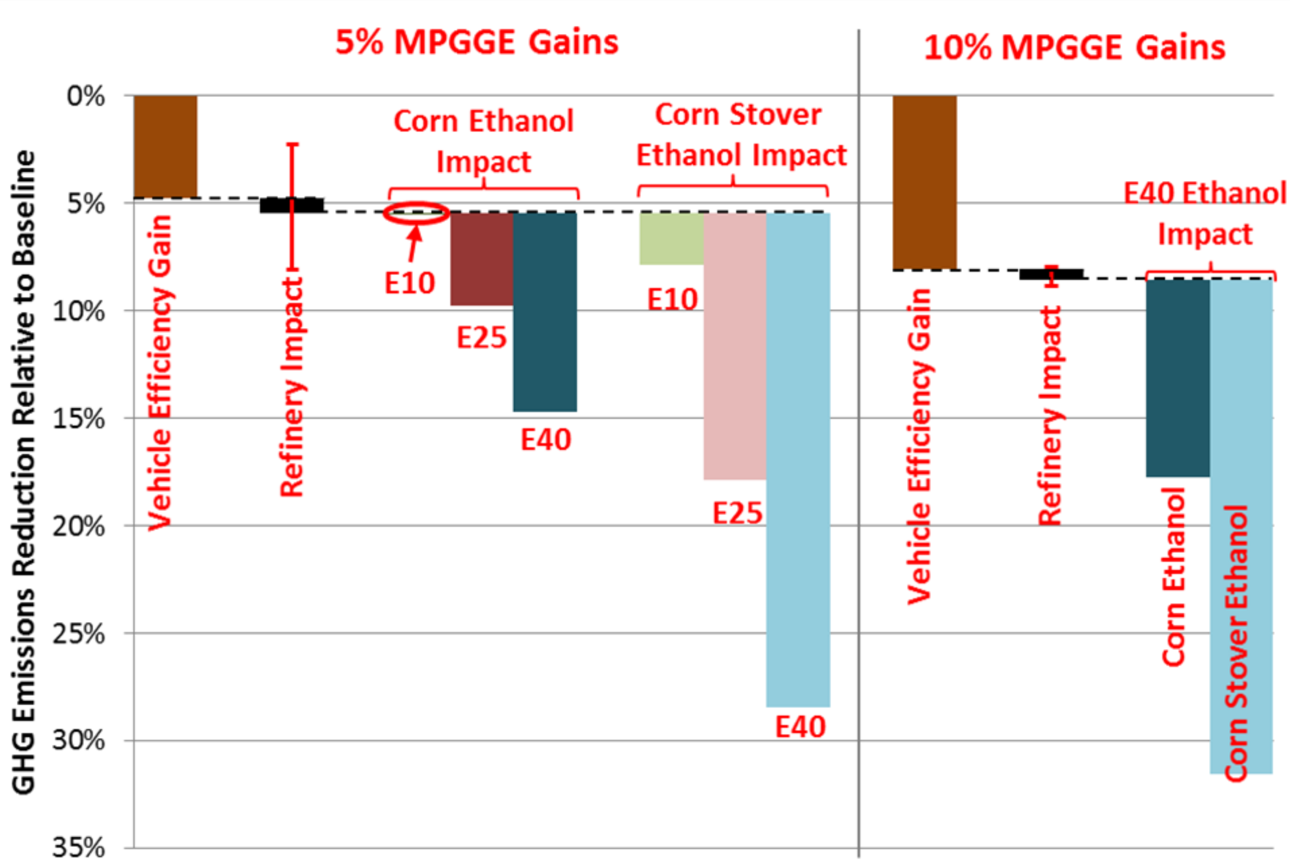
Reference	RON	Efficiency Gain (%)		Comment
		Engine	Vehicle	
Nakata et al. (2007)	**100**	7.4		Constant load, Compression ratio = 13
Leone et al. (2014)	**102**		**5.5–8.8**	Compression ratio = 13
Hirshfeld et al. (2014)			**6–9**	Compression ratio =13
Speth et al. (2014)	**98**		**3.0–4.5**	
This study	**100**		**5**	We considered **10%** for E40 as a sensitivity case

Vehicle fuel economy gains provides additional WTW GHG emissions reduction (per mile result, PADD3)



- E10, E25 and E40 HOF → 5% MPGGE gain (volumetric fuel parity at E25)
- E40 HOF Maximum → 10% MPGGE gain (Volumetric fuel parity at E40)

Effects of vehicle efficiency and ethanol blend on WTW results



- GHG reduction w/ vehicle efficiency gain: 4% with 5% MPGGE gain, 8% with 10% MPGGE gain
- Refinery BOB GHG Impact: <1%
- Ethanol Blending GHG Impact
  - Corn Ethanol: 0% for E10, 5% for E25, 10% for E40
  - Corn Stover Ethanol: 3% for E10, 12% for E25, 24% for E40

Conclusions

- Vehicle efficiency gains and ethanol blending are the two dominant factors for WTW GHG emissions reduction
- Impacts of HOF production on refinery GHG emissions is relatively small
- Ethanol can be a major enabler in producing HOF with significant vehicle efficiency gains and a large reduction in WTW GHG emissions

Outstanding issues

- Petroleum refinery LP modeling
  - RFG vs. CG: RVP 1 psi waiver only for E10 CG in summer (June 1-Sept. 30; federal); states have additional RVP requirements outside of fed RVP requirement
  - Tier 3 gasoline specs may impact HOF production
  - Crude types and natural gasoline inputs to refineries
  - Gasoline export: quality difference in domestic BOB and exported gasoline property; quantity; discounting in price
  - Capital expansion: not included in Phase 1, but being addressed in Phase 2
- Blending properties of BOB and ethanol
  - RVP curve; RVP with ethanol blends are a key issue; sensitivity analysis of 1 psi waiver in LP modeling
  - RON curve
- Other biofuels besides ethanol for HOFs? renewable gasoline, naphtha, etc.?