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Supplementary Materials

Beyond Waste: Future Sustainable Insights for Integrating Complex Feedstocks into the Global Energy Mix

The Supplementary Materials section presents methodology, calculation formulas, and initial and raw data on the methodology and theoretical calculation for diesel cost reduction for the analyses discussed in the main text (Section 1. Introduction), initial and raw data for the PRELIM model, and methodology and results for comparative economic and emissions analysis of refinery configurations with alternative hydrogen feedstocks, both discussed in the main text (Section 6. System-Level Climate Impacts and Life Cycle Perspectives). The supplementary material includes details that complement the findings reported in the main text.

Part 1. Methodology and Theoretical Calculation for Diesel Cost Reduction

The standard yield for diesel from a 42-gallon barrel of crude oil is approximately 11.5 gallons or 27.4% by volume [4]. We model the scenario of increasing this yield by an absolute change of 1% and 5%, representing new yields of 11.615 and 12.075 gallons per barrel, respectively.

The theoretical change in production cost was calculated based on the following key assumptions:

- Baseline crude cost: USD 90/barrel.
- Low-value feedstock: the additional diesel is produced by converting heavy fuel oil (HFO), valued at USD 60/barrel (USD 1.43/gallon) [5].
- Conversion cost: an incremental refining cost of USD 5/barrel for the conversion process [6].

The cost impact is derived from the opportunity cost of the lost HFO and the added conversion cost, allocated over the new, larger volume of diesel.

- Calculation for 1% yield increase

Additional diesel: calculated as 0.115 gallons/barrel.

Opportunity cost (lost HFO): calculated as 0.115 gal * USD 1.43/gal = USD 0.164/barrel.

Added conversion cost: (USD 5/barrel/42 gal/barrel) * 0.115 gal = USD 0.014/barrel.

Total added cost/barrel: USD 0.164 + USD 0.014 = USD 0.178.

Cost reduction per gallon of diesel: USD 0.178/11.615 gal ≈ USD 0.015/gal.

- Calculation for 5% yield increase

Additional diesel: calculated as 0.575 gallons/barrel.

Opportunity cost (lost HFO): calculated as 0.575 gal * USD 1.43/gal = USD 0.822/barrel.

Added conversion cost: (USD 5/barrel / 42 gal/barrel) * 0.575 gal = USD 0.068/barrel.

Total added cost/barrel: USD 0.822 + USD 0.068 = USD 0.890.

Cost reduction per gallon of diesel: USD 0.890 / 12.075 gal ≈ USD 0.074/gal.

- Market-level analysis and feedback effects

The theoretical cost benefits calculated are contingent on a ceteris paribus assumption that does not hold at a systemic level. The refining industry is governed by the equilibrium of supply and demand for individual products [7].

- Impact on crack spreads

A systemic increase in diesel yield of 5% would create a significant surplus of diesel and a corresponding deficit of other products, most notably gasoline. This would trigger immediate price adjustments in the market:

Diesel crack spread: would contract due to the supply surplus.

Gasoline crack spread: would expand due to the supply shortage.

For illustration, if the diesel crack spread fell from USD 35/barrel to USD 25/barrel, the price impact (-USD 10/barrel/42 gal/barrel ≈ -USD 0.24/gal) would completely overwhelm the theoretical USD 0.074/gal engineering cost saving.

- Scenario dependence

The economic outcome is highly scenario-dependent:

Ideal case (converting low-value products): as modeled, converting HFO is the most profitable path and can provide a marginal, temporary cost advantage.

Sub-optimal case (converting high-value products): if the yield shift is achieved by sacrificing gasoline production, and the gasoline crack spread is higher than diesel's, the refinery experiences an immediate economic loss, increasing its cost base.

While refinery process optimization to increase diesel yield can offer marginal theoretical cost reductions (e.g., ~USD 0.07/gal for a 5% yield increase), these are engineering estimates that do not account for market price elasticity.

Part 2. Initial data on hydroconversion (PRELIM model input) and raw data from PRELIM model

The open-source Petroleum Refinery Life Cycle Inventory Model (PRELIM, version 1.6) was applied with a gate-to-gate refinery boundary for estimating energy use and environmental releases from crude refining [12,86]. PRELIM standard outputs focus on refinery operations and do not

include upstream crude extraction and transport. Allocation of energy use and emissions to products follows an energy-based allocation consistent with PRELIM settings. The modeled configuration represents a deep-conversion coking refinery with deep-conversion hydroconversion refinery. Electricity and steam pathways were selected based on PRELIM default global average energy mixes and on-site natural gas-fired utilities. The initial and raw data and results of calculations via PRELIM are presented below.

Table S1. Mass balance of hydroconversion process with recycle (process parameters: catalyst concentration—0.05 %wt Mo, P=7.0 MPa, T=445^{0}C, H_2: feed=1000 nL/L, LHSV=1 h^{-1}). .

Stream	% wt.
Input	
VR	66,0
Recycle (with recycled catalyst)	29,5
H_2 consumption	2,4
Water deionized	2,0
Precursor $(NH_4)_6Mo_7O_{24}{\cdot}4H_2O$	0,1
Total input	100,0
Output	
Raw gaseous products (C_1-C_4, H_2S, NH_3)	3.8
Distillates, including the following:	89.7
IBP–180°C	14.5
180–350°C	36.7
350–520°C	38.5
Residue 520°C+, including catalyst	6.50
Total output	100.0

Table S2. Characteristics of hydroconversion products (process parameters: catalyst concentration—0.05 wt% Mo, P=7.0 MPa, T=445^{0}C, H_2: feed=1000 nL/L, LHSV=1 h^{-1}).

Property	Naphta (IBP–180°C)	Diesel (180–350°C)	Gasoil (350–520°C)	Residue (520°C+)
Density at 20 °C, kg/m³	770	871	955	1075
Elemental composition, wt%				
Carbon (C)	85,3	85,2	85,5	84,5
Hydrogen (H)	13,9	12,5	10,6	8,9
Sulfur (S)	0,6	1,9	3,1	4,9
Nitrogen (N)	0,02	0,2	0,5	1,0
Oxygen (O)	0,2	0,2	0,3	0,7

Table S3. Emission factors (gCO_2e/MJ) used in PRELIM model.

Source	Value
Electricity	152,5
Natural gas upstream	10,8
Natural gas combustion	58,4
Hydrogen via SMR	91,0

Table S4. Properties for crude assay used in PRELIM model.

		Cutoff Temp [°C]	525+
Property		Full Crude	VR
Vol flow	bpd	100 029,71	17 074,54
Vol flow	m^3/d	15 898,73	2 714,63
Mass flow	kg/d	13 722 289,22	2 767 838,04
Sulphur	wt%	1,96	4,7
Nitrogen	mass ppm	1 049,88	3 984,78
API gravity	°API	31,68	6,74
Density	kg/m^3	863,11	1 019,60
Hydrogen	wt%	12,75	10,77
MCR	wt%	3,78	18

Table S5. Results for coking refinery, "gray" H_2 (via PRELIM).

Per bbl of Crude	Energy Use and Environmental Impact									
	Energy Use	GWP	Acidification	Particulate Matter Formation	Eutrophication	Ozone Depletion	Smog	Human Health, Cancer	Human Health, Non-Cancer	Ecotoxicity
	(MJ)	(kg CO2eq)	(kg SO2eq)	(kg PM2.5eq)	(kg Neq)	(kg CFC-11eq)	(kg O3eq)	(CTUcancer)	(CTUnoncancer)	(CTUeco)
Electricity	23,21	3,57	2,80E-03	2,00E-04	1,80E-04	0,00E+00	1,00E-01	0,00E+00	0,00E+00	0,00E+00
Heat	341,8	26,26	2,00E-02	2,40E-03	8,80E-04	1,80E-08	4,90E-01	1,20E-09	9,00E-08	1,10E-02
Heat (natural gas)	341,8	23,65	1,90E-02	2,20E-03	8,30E-04	1,70E-08	4,60E-01	1,10E-09	8,20E-08	9,90E-03
Steam	28,66	2	1,60E-03	1,90E-04	7,10E-05	1,40E-09	3,90E-02	8,80E-11	6,80E-09	8,30E-04
Steam (natural gas)	28,52	1,97	1,60E-03	1,90E-04	7,00E-05	1,40E-09	3,90E-02	8,80E-11	6,80E-09	8,30E-04
Steam (electricity)	0,14	0,02	1,70E-05	1,20E-06	1,10E-06	0,00E+00	6,20E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via SMR	59,13	4,57	1,80E-03	1,20E-04	6,80E-05	2,70E-10	3,90E-02	1,70E-11	1,30E-09	1,60E-04
Steam natural gas	-0,34	-0,02	-2,00E-05	-2,30E-06	-8,40E-07	-1,70E-11	-4,70E-04	-1,10E-12	-8,30E-11	-1,00E-05
Steam electricity	0,37	0,06	4,60E-05	3,10E-06	2,90E-06	0,00E+00	1,60E-03	0,00E+00	0,00E+00	0,00E+00
Natural gas, heat SMR	5,84	0,4	3,30E-04	3,80E-05	1,40E-05	2,90E-10	7,90E-03	1,80E-11	1,40E-09	1,70E-04
Natural gas, feed SMR	53,26	0,57	1,40E-03	8,50E-05	5,20E-05	0,00E+00	3,00E-02	0,00E+00	0,00E+00	0,00E+00
SMR process emissions	-	3,56	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via catalytic naphtha reformer (CNR)	59,82	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Other emissions	36,55	4,04	4,00E-03	1,30E-03	3,70E-04	1,00E-07	6,00E-02	2,20E-09	1,70E-07	9,90E-01
FCC cat. regeneration	36,55	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Subprocess emissions	-	3,49	1,70E-03	6,10E-04	3,40E-04	1,50E-08	1,80E-02	1,40E-09	2,00E-08	4,90E-01
Support services emissions	-	0,55	2,20E-03	6,60E-04	3,30E-05	8,60E-08	4,20E-02	6,50E-10	1,40E-07	1,70E-01
Releases from managed wastes	-	0	1,00E-07	1,20E-11	4,80E-07	0,00E+00	1,10E-05	1,00E-10	4,10E-09	3,30E-01

Total refinery processes	549,17	40,43	3,10E-02	4,20E-03	1,60E-03	1,20E-07	7,30E-01	3,40E-09	2,70E-07	1,00E+00

Table S6. Results for hydroconversion refinery, "gray" H_2 (via PRELIM).

Per bbl of Crude	Energy Use and Environmental Impact									
	Energy Use	GWP	Acidification	Particulate Matter Formation	Eutrophication	Ozone Depletion	Smog	Human Health, Cancer	Human Health, Non-Cancer	Ecotoxicity
	(MJ)	(kg CO2eq)	(kg SO2eq)	(kg PM2.5eq)	(kg Neq)	(kg CFC-11eq)	(kg O3eq)	(CTUcancer)	(CTUnoncancer)	(CTUeco)
Electricity	25,93	3,99	3,20E-03	2,20E-04	2,00E-04	0,00E+00	1,10E-01	0,00E+00	0,00E+00	0,00E+00
Heat	349,02	27,19	2,10E-02	2,50E-03	9,10E-04	1,90E-08	5,00E-01	1,20E-09	9,30E-08	1,10E-02
Heat (natural gas)	349,02	24,15	2,00E-02	2,30E-03	8,50E-04	1,70E-08	4,70E-01	1,10E-09	8,40E-08	1,00E-02
Steam	26,71	1,86	1,50E-03	1,80E-04	6,60E-05	1,30E-09	3,70E-02	8,20E-11	6,40E-09	7,70E-04
Steam (natural gas)	26,57	1,84	1,50E-03	1,70E-04	6,50E-05	1,30E-09	3,60E-02	8,20E-11	6,40E-09	7,70E-04
Steam (electricity)	0,13	0,02	1,60E-05	1,10E-06	1,00E-06	0,00E+00	5,80E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via SMR	76	5,88	2,30E-03	1,60E-04	8,70E-05	3,50E-10	5,00E-02	2,20E-11	1,70E-09	2,00E-04
Steam natural gas	-0,44	-0,03	-2,50E-05	-2,90E-06	-1,10E-06	-2,20E-11	-6,00E-04	-1,40E-12	-1,10E-10	-1,30E-05
Steam electricity	0,48	0,07	5,90E-05	4,00E-06	3,70E-06	0,00E+00	2,10E-03	0,00E+00	0,00E+00	0,00E+00
RFG, heat SMR	0	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Natural gas, heat SMR	7,51	0,52	4,30E-04	4,90E-05	1,80E-05	3,70E-10	1,00E-02	2,30E-11	1,80E-09	2,20E-04
Natural gas, feed SMR	68,45	0,74	1,80E-03	1,10E-04	6,60E-05	0,00E+00	3,90E-02	0,00E+00	0,00E+00	0,00E+00
SMR process emissions	-	4,58	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,30E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via CNR	61,73	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Other emissions	42,1	4,6	4,30E-03	1,40E-03	3,90E-04	1,00E-07	6,30E-02	2,20E-09	1,70E-07	1,00E+00

FCC cat. regeneration	42,1	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Subprocess emissions	-	4,05	2,00E-03	7,10E-04	3,50E-04	1,70E-08	2,10E-02	1,50E-09	2,10E-08	4,90E-01
Support services emissions	-	0,55	2,20E-03	6,60E-04	3,30E-05	8,60E-08	4,20E-02	6,50E-10	1,40E-07	1,70E-01
Releases from managed wastes	-	0	1,00E-07	1,20E-11	4,80E-07	0,00E+00	1,10E-05	1,00E-10	4,10E-09	3,30E-01
Total Refinery processes	581,49	43,51	3,20E-02	4,40E-03	1,60E-03	1,20E-07	7,70E-01	3,50E-09	2,70E-07	1,00E+00

Table S7. Results for hydroconversion refinery, "blue" H_2 (via PRELIM).

Per bbl of Crude	Energy Use and Environmental Impact									
	Energy Use	GWP	Acidification	Particulate Matter Formation	Eutrophication	Ozone Depletion	Smog	Human Health, Cancer	Human health, Non-Cancer	Ecotoxicity
	(MJ)	(kg CO2eq)	(kg SO2eq)	(kg PM2.5eq)	(kg Neq)	(kg CFC-11eq)	(kg O3eq)	(CTUcancer)	(CTUnoncancer)	(CTUeco)
Electricity	25,93	3,99	3,20E-03	2,20E-04	2,00E-04	0,00E+00	1,10E-01	0,00E+00	0,00E+00	0,00E+00
Heat	349,02	27,19	2,10E-02	2,50E-03	9,10E-04	1,90E-08	5,00E-01	1,20E-09	9,30E-08	1,10E-02
Heat (natural gas)	349,02	24,15	2,00E-02	2,30E-03	8,50E-04	1,70E-08	4,70E-01	1,10E-09	8,40E-08	1,00E-02
Steam	26,71	1,86	1,50E-03	1,80E-04	6,60E-05	1,30E-09	3,70E-02	8,20E-11	6,40E-09	7,70E-04
Steam (natural gas)	26,57	1,84	1,50E-03	1,70E-04	6,50E-05	1,30E-09	3,60E-02	8,20E-11	6,40E-09	7,70E-04
Steam (electricity)	0,13	0,02	1,60E-05	1,10E-06	1,00E-06	0,00E+00	5,80E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via SMR	76	1,32	2,30E-03	1,60E-04	8,70E-05	3,50E-10	5,00E-02	2,20E-11	1,70E-09	2,00E-04
Steam natural gas	-0,44	-0,03	-2,50E-05	-2,90E-06	-1,10E-06	-2,20E-11	-6,00E-04	-1,40E-12	-1,10E-10	-1,30E-05
Steam electricity	0,48	0,07	5,90E-05	4,00E-06	3,70E-06	0,00E+00	2,10E-03	0,00E+00	0,00E+00	0,00E+00
Natural gas, heat SMR	7,51	0,52	4,30E-04	4,90E-05	1,80E-05	3,70E-10	1,00E-02	2,30E-11	1,80E-09	2,20E-04
Natural gas, feed SMR	68,45	0,74	1,80E-03	1,10E-04	6,60E-05	0,00E+00	3,90E-02	0,00E+00	0,00E+00	0,00E+00
SMR process emissions	-	0,02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,30E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via CNR	61,73	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Other emissions	42,1	4,6	4,30E-03	1,40E-03	3,90E-04	1,00E-07	6,30E-02	2,20E-09	1,70E-07	1,00E+00
FCC cat. regeneration	42,1	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Subprocess emissions	-	4,05	2,00E-03	7,10E-04	3,50E-04	1,70E-08	2,10E-02	1,50E-09	2,10E-08	4,90E-01
Support services emissions	-	0,55	2,20E-03	6,60E-04	3,30E-05	8,60E-08	4,20E-02	6,50E-10	1,40E-07	1,70E-01
Releases from managed wastes	-	0	1,00E-07	1,20E-11	4,80E-07	0,00E+00	1,10E-05	1,00E-10	4,10E-09	3,30E-01
Total refinery processes	581,49	38,95	3,20E-02	4,40E-03	1,60E-03	1,20E-07	7,70E-01	3,50E-09	2,70E-07	1,00E+00

Table S8. Results for hydroconversion refinery, "green" H_2 (via PRELIM).

Per bbl of Crude	Energy Use and Environmental Impact									
	Energy Use	GWP	Acidification	Particulate Matter Formation	Eutrophication	Ozone Depletion	Smog	Human Health, Cancer	Human Health, Non-Cancer	Ecotoxicity
	(MJ)	(kg CO2eq)	(kg SO2eq)	(kg PM2.5eq)	(kg Neq)	(kg CFC-11eq)	(kg O3eq)	(CTUcancer)	(CTUnoncancer)	(CTUeco)
Electricity	25,93	3,99	3,20E-03	2,20E-04	2,00E-04	0,00E+00	1,10E-01	0,00E+00	0,00E+00	0,00E+00
Heat	349,02	27,19	2,10E-02	2,50E-03	9,10E-04	1,90E-08	5,00E-01	1,20E-09	9,30E-08	1,10E-02
Heat (natural gas)	349,02	24,15	2,00E-02	2,30E-03	8,50E-04	1,70E-08	4,70E-01	1,10E-09	8,40E-08	1,00E-02
Steam	26,71	1,86	1,50E-03	1,80E-04	6,60E-05	1,30E-09	3,70E-02	8,20E-11	6,40E-09	7,70E-04
Steam (natural gas)	26,57	1,84	1,50E-03	1,70E-04	6,50E-05	1,30E-09	3,60E-02	8,20E-11	6,40E-09	7,70E-04
Steam (electricity)	0,13	0,02	1,60E-05	1,10E-06	1,00E-06	0,00E+00	5,80E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via SMR	76	0,5	2,30E-03	1,60E-04	8,70E-05	3,50E-10	5,00E-02	2,20E-11	1,70E-09	2,00E-04
Steam natural gas	-0,44	-0,03	-2,50E-05	-2,90E-06	-1,10E-06	-2,20E-11	-6,00E-04	-1,40E-12	-1,10E-10	-1,30E-05
Steam electricity	0,48	0,07	5,90E-05	4,00E-06	3,70E-06	0,00E+00	2,10E-03	0,00E+00	0,00E+00	0,00E+00
Natural gas, heat SMR	7,51	0,52	4,30E-04	4,90E-05	1,80E-05	3,70E-10	1,00E-02	2,30E-11	1,80E-09	2,20E-04
Natural gas, feed SMR	68,45	0,74	1,80E-03	1,10E-04	6,60E-05	0,00E+00	3,90E-02	0,00E+00	0,00E+00	0,00E+00
SMR process emissions	-	-0,8	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,30E-04	0,00E+00	0,00E+00	0,00E+00
Hydrogen via CNR	61,73	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Other emissions	42,1	4,6	4,30E-03	1,40E-03	3,90E-04	1,00E-07	6,30E-02	2,20E-09	1,70E-07	1,00E+00
FCC cat. regeneration	42,1	0	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Subprocess emissions	-	4,05	2,00E-03	7,10E-04	3,50E-04	1,70E-08	2,10E-02	1,50E-09	2,10E-08	4,90E-01
Support services emissions	-	0,55	2,20E-03	6,60E-04	3,30E-05	8,60E-08	4,20E-02	6,50E-10	1,40E-07	1,70E-01
Releases from managed wastes	-	0	1,00E-07	1,20E-11	4,80E-07	0,00E+00	1,10E-05	1,00E-10	4,10E-09	3,30E-01
Total refinery processes	581,49	38,13	3,20E-02	4,40E-03	1,60E-03	1,20E-07	7,70E-01	3,50E-09	2,70E-07	1,00E+00

Part 3. Comparative Economic and Emissions Analysis of Refinery Configurations with Alternative Hydrogen Feedstocks

This analysis compares the operating costs and net values for products of two refinery configurations (Scenario A and Scenario B) under different hydrogen production pathways.

The data below provides base-year (2025) values for natural gas, electricity, hydrogen, and product prices, drawn from referenced market reports and energy outlooks [93-93]. These values represent estimates; uncertainty margins (e.g., ±15% for energy prices) are acknowledged but not explicitly modeled due to the illustrative nature of the analysis. Year-specific assumptions are justified based on recent energy market projections and are clearly cited.

- Inputs and assumptions

Prices for key energy inputs

- Electricity: average industrial electricity prices by the end of 2015 are assumed to be 0.0832 USD/kWh based on historical pricing data and forecast for the United States [93].
- Natural gas: according to [94, 95], Henry Hub natural gas spot prices lie in the range **of** 2.91–3.10 USD/MMBtu. We selected a representative assumption of USD 3.10/MMBtu as a conservative, mid-range 2025 gas price for our analysis.

Hydrogen: grey hydrogen production via steam methane reforming typically costs on the order of 1.5 USD/kg, consistent with typical costs around 1-2 USD/kg [96, 97]. Adding carbon capture and storage increases costs for hydrogen, making 2.5 USD/kg a representative benchmark for blue hydrogen. Renewable hydrogen produced via water electrolysis (green hydrogen) remains significantly more expensive, with cost over 5 USD/kg as a representative current value [97].

Prices for products

Indicative mid-range prices for refined products and by-products were selected to represent a consistent internal pricing scenario for comparative assessment. Values are not intended to reproduce any specific market quotation but, rather, to reflect typical relative price relationships among refinery products in the context of 2025 [98]:

- Gasoline: USD 2.40/gal;
- Jet fuel: USD 2.80/gal;
- Ultra-low-sulfur diesel: USD 3.00/gal;
- Naphtha: USD 85/bbl;

- Fuel oil (HSFO 3.5%): USD 70/bbl;
- Refinery fuel gas: priced as natural gas equivalent;
- Petroleum coke (fuel-grade): USD 120/ton;
- Sulfur: USD 120/ton;
- Asphalt/road oil: USD 650/ton;
- Lubricants/base oils: USD 200/bbl;
- BTX aromatics (mixed): USD 1,000/ton;
- Vacuum gas oil (VGO): USD 82/bbl.

Physical assumptions for conversions

- Crude density = 0.86 kg/l = 136.7 kg/bbl;
- Product densities (typical, kg/l): gasoline, 0.74; naphtha, 0.70; jet, 0.80; ultra-low-sulfur diesel (ULSD), 0.84; fuel oil, 0.97; lubricants, 0.88; VGO, 0.90.

Calculation Formulas

Energy Cost per barrel

The total operating energy cost per barrel of crude processed for a given scenario is calculated as the sum of the costs from natural gas, electricity, and hydrogen.

$$\text{Energy Cost}_{\text{total}} = \text{Cost}_{\text{NG}} + \text{Cost}_{\text{Elec}} + \text{Cost}_{\text{H}_2} \quad \text{(S1)}$$

where:

- Cost_{NG} = Natural Gas Intensity (MMBtu/bbl) × Natural Gas Price ($/MMBtu)
- $\text{Cost}_{\text{Elec}}$ = Electricity Intensity (kWh/bbl) × Electricity Price ($/kWh)
- Cost_{H_2} = Hydrogen Intensity (kg/bbl) × Hydrogen Cost ($/kg)

Net value per barrel

The net value (NV) per barrel represents the total market value of all products yielded from one barrel of crude.

$$\text{NV} = \sum_{i=1}^{n} (\text{Mass Yield}_i \text{ (kg/bbl)} \times \text{Product Price}_i \text{ (\$/kg)}) \quad \text{(S2)}$$

Note: Product prices, typically quoted in volumetric or mass units (e.g., USD/gal, USD/bbl, USD/ton), are converted to USD/kg for this calculation using standard product densities.

Netback per barrel

The netback is the net value remaining after accounting for operating costs. Two levels of netback are calculated:

a) Energy-only netback:

$$\text{Netback}_{\text{energy-only}} = \text{NV} - \text{Energy Cost}_{\text{total}} \quad \text{(S3)}$$

b) Full cost netback (including assumed non-energy costs):

$$\text{Netback}_{\text{full cost}} = \text{NV} - \text{Energy Cost}_{\text{total}} \quad \text{(S4)}$$

The incremental netback for Scenario B versus the baseline Scenario A is:

$$\Delta\text{Netback} = \text{Netback}_B - \text{Netback}_A \quad \text{(S5)}$$

Marginal abatement cost (MAC)

The marginal abatement cost represents the cost (or savings) associated with avoiding one ton of CO_2-equivalent emissions by adopting a lower-emission scenario (B) over the baseline (A).

$$\text{MAC (\$/tCO}_2\text{eq)} = \frac{\Delta\text{Netback (\$/bbl)}}{\Delta\text{GHG (tCO}_2\text{eq/bbl)}} \quad \text{(S6)}$$

where:

- ΔNetback is the incremental netback of Scenario B vs. A (from above).
- $\Delta\text{GHG} = \text{GHG}_A - \text{GHG}_B$ is the absolute emissions abatement (converted from kg/bbl to t/bbl).

A negative MAC value indicates a cost-saving abatement opportunity, while a positive MAC indicates a net cost to abate emissions.

Carbon price Impact on Savings

The per-barrel savings (or cost) induced by a specific carbon price P_{CO_2} are calculated as:

$$\text{Savings}_{\text{carbon}} \text{(\$/bbl)} = P_{CO_2} \text{(\$/tCO}_2\text{eq)} \times \Delta\text{GHG (tCO}_2\text{eq/bbl)} \quad \text{(S7)}$$

- Energy cost per barrel analysis

The operating energy cost for two refinery configurations (Scenario A and Scenario B) is calculated based on the process energy and hydrogen intensities per barrel of crude obtained from results provided by the PRELIM model:

Table S9. Process input intensities per barrel of crude.

Input	Scenario A	Scenario B
Natural gas (MMBtu/bbl)	0.3511	0.3561
Electricity (kWh/bbl)	6.44	7.19
Hydrogen (kg/bbl)	0.4925	0.6333

The resulting energy costs for each scenario are broken down below.

Table S10. Energy cost breakdown (USD/bbl).

Scenario	Natural gas	Electricity	Hydrogen	Total
A (gray H_2)	USD 1.30	USD 0.58	USD 0.74	USD 2.62
B (gray H_2)	USD 1.32	USD 0.65	USD 0.95	USD 2.92
B (blue H_2)	USD 1.32	USD 0.65	USD 1.58	USD 3.55
B (green H_2)	USD 1.32	USD 0.65	USD 3.17	USD 5.14

- Net value per barrel

Using mass-based yields and the established product prices, the net value (NV) per barrel of crude was calculated.

- Scenario A (gray H_2) NV**:** USD 105.60/bbl
- Scenario B (gray H_2) NV**:** USD 108.32/bbl
- Incremental net value (Scenario B-Scenario A)**:** +USD 2.72/bbl

The +USD 2.72/bbl uplift in Scenario B is attributed to the following dominant effects:

Higher yield of light/middle distillates**:** gasoline (+USD 1.06), ULSD (+USD 0.90), naphtha (+USD 0.52), jet fuel (+USD 0.25).

Increased low-value streams**:** fuel gas (+USD 0.19), fuel oil (+USD 0.44).

Reduced low-value revenue**:** removal of coke reduces revenue (-USD 0.66).

Minor contributions**:** BTX (+USD 0.14), sulfur (+USD 0.03), VGO (-USD 0.16).

- Netbacks and marginal abatement cost

Netback analysis

The netback is defined as the net value minus (operating) energy costs.

Table S11. Netback analysis (USD/bbl).

Metric	Scenario A (gray H_2)	Scenario B (gray H_2)	Scenario B (blue H_2)	Scenario B (green H_2)
Net value (NV)	USD 105.60	USD 108.32	USD 108.32	USD 108.32
Energy-only netback (= NV − energy cost)	USD 102.98	USD 105.40	USD 104.77	USD 103.18
Increment (Δ) vs. A	-	+USD 2.42	+USD 1.79	+USD 0.20

Non-energy O&M/catalyst cost* (assumed)	+USD 1.30	+USD 1.60	+USD 1.60	+USD 1.60
Full cost netback (= NV − energy cost − O&M/catalyst cost)	USD 101.68	USD 103.81	USD 103.17	USD 101.59
Increment (Δ) vs. A	-	+USD 2.13	+USD 1.49	-USD 0.09

O&M stands for operations and maintenance; catalyst—for catalyst precursor for Scenario B, numbers in table are illustrative.

Emissions and marginal abatement cost (MAC)

The system-wide GHG emissions and the resulting marginal abatement costs are calculated as follows:

Table S12. Emissions and abatement economics.

Scenario	GHG (kg CO_{2eq}/bbl)	Abatement vs. A (kg/bbl)	MAC (Energy Only) (USD/tCO_{2eq})	MAC (Incl. O&M/Catalyst) (USD/tCO_{2eq})
A (gray H_2)	96.7	-	-	-
B (gray H_2)	85.3	11.4	-212	-186
B (blue H_2)	80.7	16.0	-112	-93
B (green H_2)	79.9	16.8	-12	+6

A carbon price sensitivity analysis shows that at USD 50/tCO_{2eq}, the per-barrel savings for Scenario B versus A would be as follows:

Scenario B (gray H_2)—USD 0.57; Scenario B (blue H_2)—USD 0.80; Scenario B (green H_2)—USD 0.84.

At this carbon price, for Scenario B (green H_2), the slight positive cost with extra O&M/catalyst (+USD 0.10/bbl) would flip to a net gain of -USD 0.74/bbl.

- Summary of costs per barrel

Table S13. Consolidated cost and value overview (USD/bbl).

Scenario	Operating energy Cost	Net Value (Energy Only)*	Net Value (Incl. Energy and O&M/Catalyst)*
Scenario A (gray H_2)	2.62	102.98	101.68
Scenario B (gray H_2)	2.92	105.40	103.81
Scenario B (blue H_2)	3.55	104.77	103.17
Scenario B (green H_2)	5.14	103.18	101.59

*from Table S11.

Method Notes and Limitations

Capital expenditure exclusion: the study focuses exclusively on operating costs. The significant upfront capital investment required to build a new refinery configuration (Scenario B) or to retrofit existing facilities for blue/green hydrogen production is not considered. A full economic analysis would require a levelized cost of hydrogen (or a full lifecycle cost analysis

including capital expenditure, which could dramatically change the economics, especially for green hydrogen).

Regional specificity: these results are based on U.S.-centric 2025 midpoints. Real-world refinery economics are highly sensitive to regional tariffs, contracts for power/gas, and local product spot prices.

Price sensitivity: the entire analysis is highly sensitive to the assumed "Product Price" A sensitivity analysis. Showing how the net value and netbacks change with ±10-20% fluctuations in key product prices (e.g., diesel, gasoline) would be valuable. The relative attractiveness of scenarios can reverse with shifting market conditions.

Hydrogen cost uncertainty: the hydrogen cost midpoints (USD 1.50, USD 2.50, USD 5.00/kg) are critical inputs. The document does not discuss the uncertainty range or potential future cost reductions (e.g., for green hydrogen due to technological advances or policy support like the Inflation Reduction Act's 45V tax credit), which could fundamentally alter the conclusions.

In summary, while the document provides a robust comparative analysis of operating costs and emissions under specific conditions, a fully informed decision would require considering the excluded factors of capital costs, technology maturity, price volatility, full lifecycle emissions, and broader system-level impacts and risks.