Supporting information

An Integrated Techno-Economic Analysis and Life Cycle Assessment of Lube Oil Production from Post-Used Polypropylene and Comparison with Conventional Base Oils

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Number of Tables: 37

Number of Figures: 12

Section S1. Process modeling for lubricant base oil production from crude oil

Group I process

Crude oil is introduced to the pre-flash column at 93.33 °C and at a pressure of 4.14 bar. The bottom product of the pre-flash column, known as ATM-feed (the crude stream oil) is then directed to the atmospheric distillation column (ATM column). In the ATM column, the crude stream oil is heated to 226.7 °C at pressure of 3.08 bar. The vaporized crude is separated into heavy naphtha (H-naphtha), kerosene, diesel, atmospheric gas oil (AGO), and atmospheric residue (At-residue). The At-residue is sent to the vacuum distillation column (VD column) at 328.06 °C and a pressure of 1.70 bar. The first step in lubricant base oil production involves vacuum distillation of the atmospheric residue obtained from the bottom product of the atmospheric distillation process. The vacuum fractionator divides the atmospheric residue into light vacuum gas oil (LVGO), heavy vacuum gas oil (HVGO), and vacuum residue. The vacuum residue is at a temperature of 302.59 °C and pressure of 0.09 bar. HVGO is sent to the aromatic extraction unit, while the vacuum residue is transferred to the propane deasphalting unit. The vacuum residue contains undesirable components such as asphaltenes. To improve the quality of the produced lubricating base oils, aromatic hydrocarbons need to be extracted from the lube oil cuts (HVGO). This is achieved through a liquid-liquid extraction process. Furfural, a solvent with high enough selectivity for aromatics extraction, is widely used in this process. During solvent extraction, HVGO and furfural are thoroughly mixed to maximize the yield of extraction.

The extraction of the aromatics increases with a higher solvent-to-feed volumetric flow rate ratio and elevated feed and solvent temperatures. Solvent extraction is required to remove the aromatics from the base oil feedstocks to improve viscosity, oxidation resistance, and color.[1–3] Furfural is utilized at 31.8 °C and 0.09 bar. After the extraction, furfural is separated from the oil stream through distillation, and the extracted stream is directed to the solvent dewaxing column. The solvent dewaxing process ensures the removal of paraffins from the oil, achieving adequate viscosity at lower ambient temperatures. At first, the extracted stream is diluted with propane (solvent) to reduce viscosity, cooled down to a temperature at which wax crystallizes, and then filtered to eliminate the wax.[4] The solvent de-asphalting column is used to extract lighter paraffinic and naphthenic hydrocarbons (asphaltenes and resins) from the vacuum residue.[5] Propane is used as a solvent under operating conditions of 96.7 °C and 42.47 bar. Propane has a higher selectivity for removing resins and asphaltenes from base oil. Figure S1 illustrates the various unit operations involved in the production of Group I base oil from crude oil.

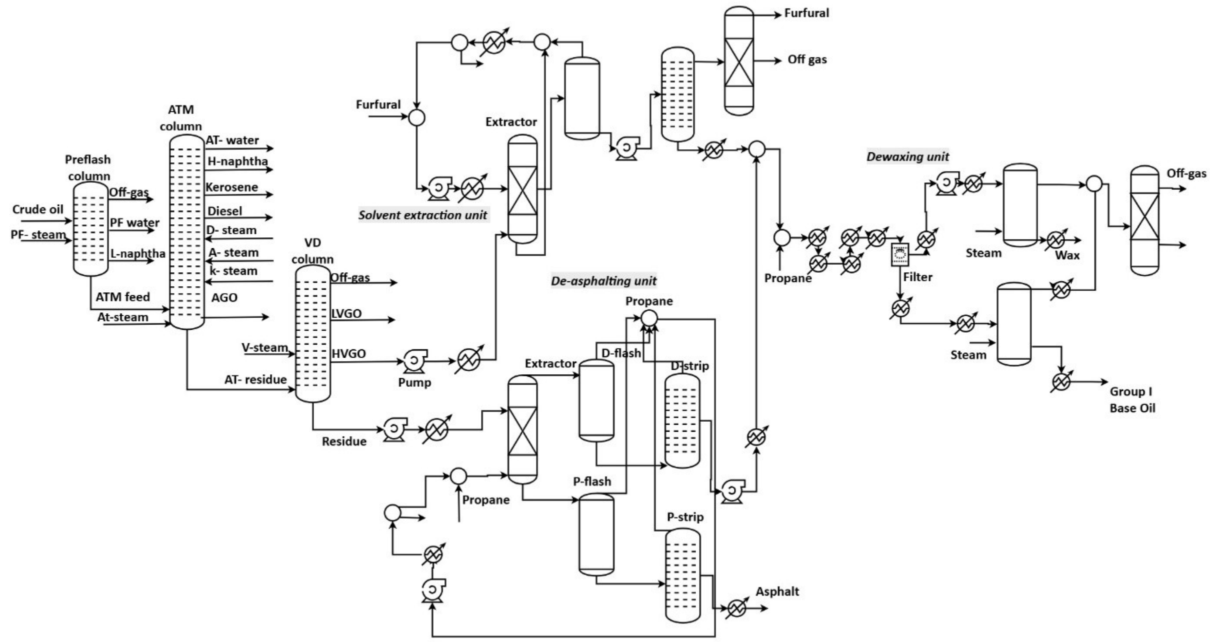

Figure S1. Simplified process flow diagram for producing Group I base oil from crude oil. ATM: Atmospheric distillation, HVGO: Heavy vacuum gas oil, LVGO: Light vacuum gas oil, VD: vacuum distillation columns.

Group II and Group III processes

Crude oil is processed through the pre-flash column, ATM column, and VD column, similar to the Group I base oil production process. HVGO and the residue of solvent de-asphalting are sent to the hydrotreating and hydrocracking columns to produce Group II and Group III base oils, respectively. Hydrotreating and hydrocracking reactions are performed at catalyst temperatures of 340.6 °C, with reactor pressures of 55.16 bar and 82.7 bar, respectively.[6] To eliminate catalyst fouling and enable long-term operations without catalyst regeneration, a large amount of hydrogen is utilized with the feedstock during hydrocracking. The catalyst employed in both hydrocracking and hydrotreating processes is cobalt molybdenum (Co-Mo/Al_2O_3), with a lifetime ranging from 2 to 4 years in industrial applications. Figures S2 and S3 display the different unit operations involved in the production of Group II and II base oils from crude oil, respectively.

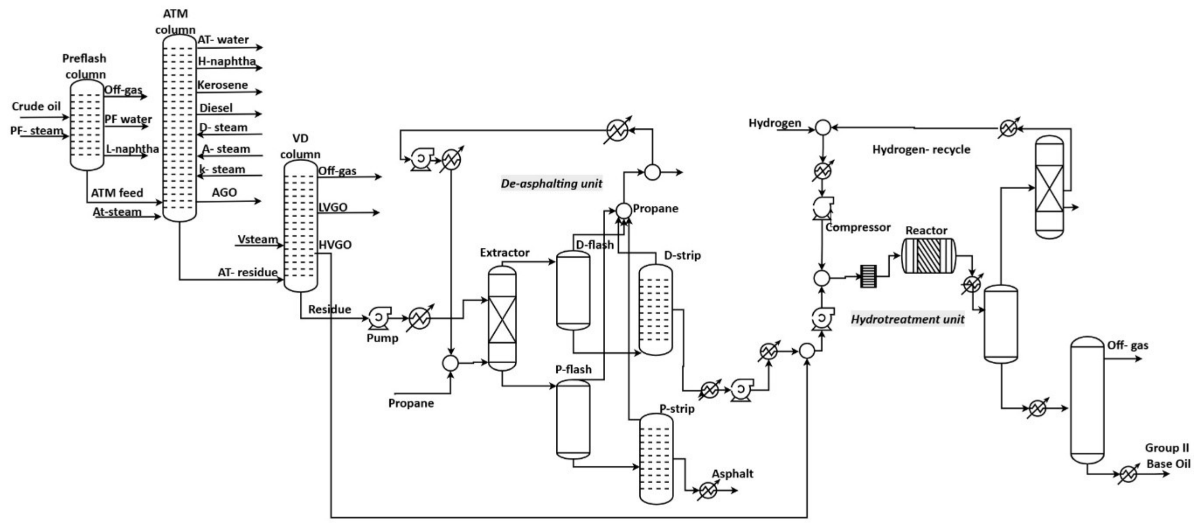

Figure S2**.** Simplified process flow diagram for producing Group II base oil from crude oil. ATM: Atmospheric distillation, HVGO: Heavy vacuum gas oil, LVGO: Light vacuum gas oil, VD: vacuum distillation columns.

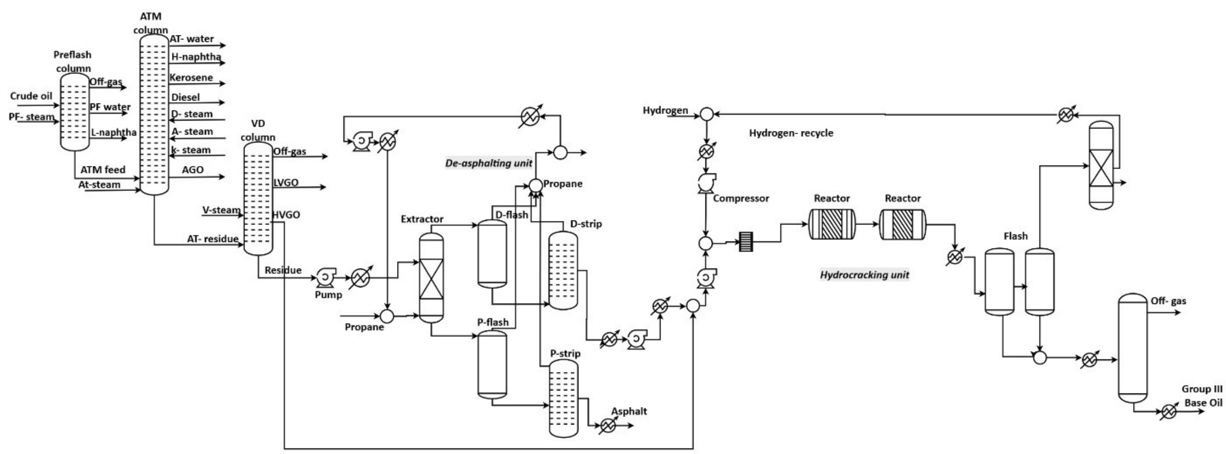

Figure S3**.** Simplified process flow diagram for producing Group III base oil from crude oil. ATM: Atmospheric distillation, HVGO: Heavy vacuum gas oil, LVGO: Light vacuum gas oil, VD: vacuum distillation columns.

The crude oil assay data are sourced from AspenTech[7] and are presented in Tables S1, S2, and S3. Through the process modeling, material inputs and outputs and energy use associated with the refining of the three base oils are estimated. Detailed data on the material flows and energy requirements at each stage of refining for Group I, Group II, and Group III base oils are presented in Tables S6, S7, and S8, respectively. This dataset served as the foundation for conducting a techno-economic analysis (TEA) and a life-cycle assessment (LCA) of the base oils, which are described in the upcoming sections.

Table S1. Basrah light crude oil assay data

True boiling point distillation (weight basis)	
Temperature (°C)	% Distilled
20	1.3
65	5.0
175	21.2
225	29.4
360	52.3
525	77.4

Table S2. Property data for Basrah light crude oil sulfur content (Weight basis)

Mid percent distilled	Sulfur content (%)
25.30	0.1
40.85	1.2
64.85	2.4
76.15	3.6
88.70	4.7

Table S3. Property data for Basrah light crude oil (API gravity)

True boiling point distillation (weight basis)	
Mid percent distilled	API gravity
3.15	87.54
13.10	60.49
25.30	46.49
40.85	36.35
64.85	22.98
76.15	14.98
88.17	7.23

Section S2: Techno-economic analysis results for lube base oil production from crude oil

Table S4. Raw materials, chemicals, and utilities costs used for the process design

Item	Cost*	Source
Diesel ($/kg)	0.68	U.S. EIA[8]
kerosene ($/kg)	0.67	U.S. EIA[9]
Propane ($/kg)	0.50	U.S. EIA[10]
Catalyst ($/kg)	300	Riogen[11]
Asphalt ($/kg)	0.69	New York State DOT[12]
Naphtha ($/kg)	0.64	Business analytiq[13]
Paraffin wax ($/kg)	1.48	Business analytiq[14]
Crude oil ($/gal)	1.85	U.S. EIA[15]
Furfural ($/kg)	1.44	Dubbink et al.[16]
Electricity ($/kWh)	0.09	U.S. EIA[17]
Natural gas ($/GJ)	4.16	U.S. EIA[18]

*Cost adjusted to the 2023 analysis base year

Table S5. Techno-economic assumptions used for the design process to produce Group I, II, and III base oils from crude oil

Parameter	
Working capital percentage (% per year)	5
Operating charges (% per year)	25
Plant overhead (% per year)	50
Desired rate of return (% per year)	10
Tax rate (% per year)	40
Plant life (years)	20
Economic life of the project (years)	20
Salvage value (Percent of initial capital cost)	20
Depreciation method	Straight line
Project capital escalation (% per year)	5
Products escalation (% per year)	5
Raw material escalation (% per year)	3.5
Operating and maintenance labor escalation (% per year)	3
Utilities escalation (% per year)	3
General and administrative expenses (% per year)	8

Material balances and energy use in different stages, operational specifications for key downstream process units, and the main equipment cost for Group I, II, and III base oils

Table S6. Material balances and energy use in the different stages for Group I base oil production

Stage	Category	Item	Flow	
Preflash column	Input streams	Crude Oil	1,132,492.92	kg/h
		Steam	2,267.96	kg/h
	Output streams	Off gas	24,200.61	kg/h
		Light naphtha	166,555.08	kg/h
		Atmospheric Column Feed	944,005.19	kg/h
	Energy use	Natural gas	500.01	GJ/h
Atmospheric distillation column	Input streams	Atmospheric Column Feed	944,005.19	kg/h
		Steam	7,756.43	kg/h
	Output streams	Water	7,699.18	kg/h
		Heavy naphtha	91,411.01	kg/h
		Kerosene	62,196.39	kg/h
		Diesel	187,136.74	kg/h
		Atmospheric gasoil	49,399.18	kg/h
		Atmospheric residue	553,919.13	kg/h
	Energy use	Natural gas	470.57	GJ/h
Vacuum distillation column	Input streams	Atmospheric residue	553,919.13	kg/h
		Steam	9,071.85	kg/h
	Output streams	Vacuum Off gas	10,011.86	kg/h
		Light vacuum gasoil	46,834.08	kg/h
		Heavy vacuum gasoil	100,416.65	kg/h
		Vacuum residue	405,728.39	kg/h
	Energy use	Natural gas	54.22	GJ/h
Solvent extraction	Input streams	Heavy vacuum gasoil	100,416.65	kg/h
		Furfural Make-up	631.32	kg/h
	Output streams	Residue	2,871.98	kg/h
		Base oil with wax	98,175.99	kg/h
	Energy use	Natural gas	234.62	GJ/h
		Electricity	0.19	GJ/h
Deasphalting	Input streams	Vacuum residue	405,728.39	kg/h
		Propane make-up	17,570.04	kg/h
	Output streams	Base oil with impurity	346,551.06	kg/h
		Asphalt	76,747.36	kg/h
	Energy use	Natural gas	29.53	GJ/h
		Electricity	4.34	GJ/h
Dewaxing	Input streams	Base oil with wax from heavy vacuum gasoil	98,175.99	kg/h
		Base oil with wax from vacuum residue	346,551.06	kg/h
		Propane make-up	4,354.01	kg/h
		Steam	1,361.32	kg/h
	Output streams	Wax	444.91	kg/h
		Group I Base oil	446,896.41	kg/h
		Residue	3,101.06	kg/h
	Energy use	Natural gas	255.74	GJ/h
		Electricity	50.19	GJ/h

Table S7. Material balances and energy use in the different stages for Group II base oil production

Stage	Category	Item	Flow	
Preflash column	Input streams	Crude Oil	566,246.46	kg/h
		Steam	2,267.96	kg/h
	Output streams	Off gas	15,921.50	kg/h
		Water	519.01	kg/h
		Light naphtha	82,840.36	kg/h
		Atmospheric Column Feed	469,233.56	kg/h
	Energy use	Natural gas	253.77	GJ/h
Atmospheric distillation column	Input streams	Atmospheric Column Feed	469,233.56	kg/h
		Steam	7,756.43	kg/h
	Output streams	Water	7,735.22	kg/h
		Heavy naphtha	42,331.28	kg/h
		Kerosene	62,867.46	kg/h
		Diesel	65,726.35	kg/h
		Atmospheric gasoil	49,509.04	kg/h
		Atmospheric residue	248,820.64	kg/h
	Energy use	Natural gas	272.21	GJ/h
Vacuum distillation column	Input streams	Atmospheric residue	248,820.64	kg/h
		Steam	9,071.85	kg/h
	Output streams	Vacuum Off gas	9,277.32	kg/h
		Light vacuum gasoil	48,861.62	kg/h
		Heavy vacuum gasoil	105,897.37	kg/h
		Vacuum residue	93,856.17	kg/h
	Energy use	Natural gas	151.50	GJ/h
Deasphalting	Input streams	Vacuum residue	93,856.17	kg/h
		Propane make-up	2,374.21	kg/h
	Output streams	Base oil with impurity	125.97	kg/h
		Asphalt	96,104.23	kg/h
	Energy use	Natural gas	9.86	GJ/h
		Electricity	1.19	GJ/h
Hydrotreatment	Input streams	Heavy vacuum gasoil	105,897.37	kg/h
		Base oil with wax	125.97	kg/h
		Hydrogen	3,237.07	kg/h
	Output streams	Off-gas	1,977.19	kg/h
		Group II Base oil	103,108.27	kg/h
		Purge	4,174.36	kg/h
	Energy use	Natural gas	459.23	GJ/h
		Electricity	456.87	GJ/h

Table S8. Material balances and energy use in the different stages for Group III base oil production

Stage	Category	Item	Flow	
Preflash column	Input streams	Crude Oil	566,246.46	kg/h
		Steam	2,267.96	kg/h
	Output streams	Off gas	15,682.25	kg/h
		Water	527.85	kg/h
		Light naphtha	84,205.64	kg/h
		Atmospheric Column Feed	468,098.68	kg/h
	Energy use	Natural gas	253.77	GJ/h
Atmospheric distillation column	Input streams	Atmospheric Column Feed	468,098.68	kg/h
		Steam	7,756.43	kg/h
	Output streams	Water	7,744.60	kg/h
		Heavy naphtha	41,205.57	kg/h
		Kerosene	62,867.88	kg/h
		Diesel	65,671.97	kg/h
		Atmospheric gasoil	49,508.25	kg/h
		Atmospheric residue	248,856.84	kg/h
	Energy use	Natural gas	272.18	GJ/h
Vacuum distillation column	Input streams	Atmospheric residue	248,856.84	kg/h
		Steam	9,071.85	kg/h
	Output streams	Vacuum Off gas	9,277.16	kg/h
		Light vacuum gasoil	48,860.31	kg/h
		Heavy vacuum gasoil	105,894.01	kg/h
		Vacuum residue	93,897.21	kg/h
	Energy use	Natural gas	151.34	GJ/h
Deasphalting	Input streams	Vacuum residue	93,897.21	kg/h
		Propane make-up	604.24	kg/h
	Output streams	Base oil with impurity	192.44	kg/h
		Asphalt	94,308.84	kg/h
	Energy use	Natural gas	276.50	GJ/h
		Electricity	1.48	GJ/h
Hydrocracking	Input streams	Heavy vacuum gasoil	105,894.01	kg/h
		Base oil with wax	192.44	kg/h
		Hydrogen	4,108.59	kg/h
	Output streams	Off-gas	343.76	kg/h
		Group III Base oil	105,757.44	kg/h
		Purge	4,093.82	kg/h
	Energy use	Natural gas	926.72	GJ/h
		Electricity	790.10	GJ/h

Table S9. Operation specifications for the key downstream process units for Group I base oil

Stage	Equipment	Item	Value
Preflash column	Pre-flash column	Number of stages	10
		Furnace temperature (°C)	232
		Furnace pressure (bar)	3.44
Atmospheric column	Atmospheric distillation column	Number of stages	25
		Stage 1/Condenser pressure (bar)	1.08
		Condenser /top stage temperature (°C)	82.20
Vacuum distillation column	Vacuum distillation column	Number of stages	6
		Stage 1/Condenser pressure (bar)	0.08
		Bottom stage pressure (bar)	0.09
Solvent extraction	Extractor	Number of stages	4
		Top stage temperature (°C)	71.38
		Bottom stage temperature (°C)	68.7
	Flash	Temperature (°C)	102.8
		Pressure (bar)	0.08
De-asphalting	RadFrac (DSTRIP)	Number of stages	4
		Top stage pressure (bar)	14.96
		Top stage/Condenser temperature (°C)	43.8
		Reboiler pressure (bar)	14.96
		Reboiler temperature (°C)	99.98
	RadFrac (PSTRIP)	Number of stages	4
		Top stage pressure (bar)	14.96
		Top stage/Condenser temperature (°C)	43.8
		Reboiler pressure (bar)	14.96
		Reboiler temperature (°C)	100.89
	Extractor	Number of stages	4
		Top stage temperature (°C)	90.58
		Bottom stage temperature (°C)	99.09
	D-flash	Temperature (°C)	100
		Pressure (bar)	15
	P-flash	Temperature (°C)	100
		Pressure (bar)	15
Dewaxing	Distillation column 1	Number of stages	3
		Top stage pressure (bar)	1
		Reboiler pressure (bar)	1
	Distillation column 2	Number of stages	3
		Top stage pressure (bar)	1
		Reboiler pressure (bar)	1

Table S10. Operation specifications for key downstream process units for Group II base oil

Stage	Equipment	Item	Value
Preflash column	Pre-flash column	Number of stages Furnace temperature (°C) Furnace pressure (bar)	10 232 3.44
Atmospheric column	Atmospheric distillation column	Number of stages Stage 1/Condenser pressure (bar) Condenser /top stage temperature (°C)	25 1.08 83.12
Vacuum column	Vacuum distillation column	Number of stages Stage 1/Condenser pressure (bar) Bottom stage pressure (bar)	6 0.08 0.09
De-asphalting	RadFrac (DSTRIP)	Top stage pressure (bar) Top stage/Condenser temperature (°C) Reboiler pressure (bar) Reboiler temperature (°C)	14.96 43.83 14.96 233.6
	RadFrac (PSTRIP)	Top stage pressure (bar) Top stage/Condenser temperature (°C) Reboiler pressure (bar) Reboiler temperature (°C)	14.96 43.82 14.96 100.9
	Extractor	Number of stages Top stage temperature (°C) Bottom stage temperature (°C)	8 95.53 97.64
	D-flash	Temperature (°C) Pressure (bar)	100 15
	P-flash	Temperature (°C) Pressure (bar)	100 15
Hydrotreatment	Compressor	Discharge pressure Efficiency	55.16 0.72
	Reactor	Reactor temperature (°C) Reactor length (m) Reactor diameter(m) Reactor residence time (s)	340.6 10 1.97 14.31
	Flash	Pressure (bar) Temperature (°C)	31.23 204.44
	Radfrac	Top stage pressure (bar) Molar reflux ratio	0.96 1.2

Table S11. Operation specifications for key downstream process units for Group III base oil

Stage	Equipment	Item	Value

Preflash column	Pre-flash column	Number of stages Furnace temperature (°C) Furnace pressure (bar)	10 232.22 3.44
Atmospheric column	Atmospheric distillation column	Number of stages Stage 1/Condenser pressure (bar) Condenser /top stage temperature (°C)	25 1.08 83.48
Vacuum column	Vacuum distillation column	Number of stages Stage 1/Condenser pressure (bar) Bottom stage pressure (bar)	6 0.08 0.09
De-asphalting	RadFrac (DSTRIP)	Number of stages Top stage pressure (bar) Top stage/Condenser temperature (°C) Reboiler pressure (bar) Reboiler temperature (°C)	10 14.96 43.83 14.96 302.29
	RadFrac (PSTRIP)	Number of stages Top stage pressure (bar) Top stage/Condenser temperature (°C) Reboiler pressure (bar) Reboiler temperature (°C)	10 14.96 43.83 14.96 852.51
	Extractor	Number of stages Top stage temperature (°C) Bottom stage temperature (°C)	8 96.5 97.92
	D-flash	Temperature (°C) Pressure (bar)	100 15
	P-flash	Temperature (°C) Pressure (bar)	100 15
Hydrocracking	Radfrac column	Number of stages Top stage pressure (bar) Reboiler pressure (bar)	10 0.97 0.97
	Compressor	Discharge pressure (bar) Efficiency	82.73 0.72
	Reactor	Reactor temperature (°C) Reactor length (m) Reactor diameter(m) Reactor residence time (s)	340.6 12 1.97 13.7
	Flash	Pressure (bar) Temperature (°C)	31.23 315.6

Table S12. Main equipment cost used for producing Group I base oil from crude oil

Stage	Main equipment	Installed cost	Sources
Preflash	Preflash column	$1,151,400	APEA[19]

	Preflash furnace	$6,332,300	APEA[19]
Atmospheric column	Atmospheric column	$2,751,600	APEA[19]
	Atmospheric furnace	$5,852,300	APEA[19]
Vacuum column	Vacuum column	$1,084,900	APEA[19]
	Vaccum furnace	$818,200	APEA[19]
Solvent extraction	Extractor	$101,900	APEA[19]
De-asphalting	RadFrac (DSTRIP)	$472,300	APEA[19]
	RadFrac (PSTRIP)	$369,700	APEA[19]
	Extractor	$101,900	APEA[19]
	D-flash	$500,600	APEA[19]
	P-flash	$251,200	APEA[19]
Dewaxing	Distillation column 1	$564,600	APEA[19]
	Distillation column 2	$3,556,500	APEA[19]

APEA: Aspen process economic analyzer v12.

Table S13. Main equipment cost used for producing Group II base oil from crude oil

Stage	Main equipment	Installed cost	Sources
Preflash column	Preflash column	$963,700	APEA[19]
	Preflash furnace	$3,766,400	APEA[19]
Atmospheric column	Atmospheric column	$2,102,600	APEA[19]
	Atmospheric furnace	$3,763,200	APEA[19]
Vacuum column	Vacuum column	$1,592,000	APEA[19]
	Vaccum furnace	$2,250,800	APEA[19]
De-asphalting	RadFrac (DSTRIP)	$407,600	APEA[19]
	RadFrac (PSTRIP)	$457,300	APEA[19]
	Extractor	$101,900	APEA[19]
	D-flash	$122,000	APEA[19]
	P-flash	$277,100	APEA[19]
Hydrotreatment	Reactor	$518,400	APEA[19]
	Compressor 1	$3,380,000	Turton et al.[20]

APEA: Aspen process economic analyzer v12.

Table S14. Main equipment cost used for producing Group III base oil from crude oil

Stage	Main equipment	Installed cost	Sources
Preflash	Preflash column	$964,100	APEA[19]

	Preflash furnace	$3,766,400	APEA[19]
Atmospheric column	Atmospheric column	$2,102,200	APEA[19]
	Atmospheric furnace	$3,762,900	APEA[19]
Vacuum column	Vacuum column	$1,591,900	APEA[19]
	Vacuum furnace	$2,248,800	APEA[19]
De-asphalting	RadFrac (DSTRIP)	$410,700	APEA[19]
	RadFrac (PSTRIP)	$306,700	APEA[19]
	Extractor	$101,900	APEA[19]
	D-flash	$157,100	APEA[19]
	P-flash	$277,100	APEA[19]
Hydrocracking unit	Reactors	$1,442,000	APEA[19]
	Radfrac column	$2,419,000	APEA[19]
	Compressor 1	$3,380,000	Turton et al.[20]

APEA: Aspen process economic analyzer v12.

Table S15. Summary of economic analysis for Group I base oil production

Investment Analysis	
Total capital cost ($)	$89,535,600
Total operating cost ($/yr)	$6,748,080,000
Total raw materials cost ($/yr)	$6,167,810,000
Co-product credits ($/yr)	$4,102,203,552
Total utilities cost ($/yr)	$77,221,300
Desired rate of return (%/yr)	10
Lube oil flow rate (kg/h)	446,896

Table S16. Summary of economic analysis for Group II base oil production

Investment Analysis	
Total capital cost ($)	$69,411,615
Total operating cost* ($/yr)	3,455,721,275
Total raw materials cost [$/yr)	$2,905,680,000
Co-product credits ($/yr)	$2,475,540,812
Total utilities cost ($/yr)	$41,275,500
Desired rate of return (%/yr)	10
Lube oil flow rate (kg/h)	103,108
Total catalyst cost ($/yr)	270,021,275

*The total operating cost includes the catalyst cost.

Table S17. Summary of economic analysis for Group III base oil production

Investment Analysis

Total capital cost ($)	$80,885,490
Total operating cost* ($/yr)	$3,883,500,437
Total raw materials cost ($/yr)	$2,920,310,000
Co-product credits ($/yr)	$2,548,025,633
Total utilities cost ($/yr)	$45,869,000
Desired rate of return (%/yr)	10
Lube oil flow rate (kg/h)	105,757
Total catalyst cost ($/yr)	$676,850,437

*The total operating cost includes the catalyst cost.

Section S3. Techno-economic analysis results for lubricating oils from upcycled plastics (LOUPs) production from post-use polypropylene (PU-PP)

Table S18. Process modeling parameters for LOUPs production

Operating Conditions	
Reactor temperature (°C)	310
Reactor pressure (bar)	14.80
Hydrogen gas	100%
Reactor outputs	Gaseous products: methane, ethane, propane, butane, pentane, hexane, heptane, octane, nonane Liquid product: Lube oil

Table S19. Raw materials, chemicals, and utilities costs for the design process

Item	Cost*	Source
Process water ($/tonne)	0.60	Davis et al.[21]
Hydrogen ($/kg)	2.25	Davis et al.[21]
PU-PP ($/kg)	0.38	Resource Plastics[22] and Resource Recycling[23]
Hexane ($/kg)	1.02	ChemCatBio[24]
Electricity ($/kWh)	0.09	U.S. EIA[17]
Natural gas ($/GJ)	4.16	U.S. EIA[18]

*Cost adjusted to the 2023 analysis base year

Table S20. Techno-economic assumptions used for the design process to produce LOUPs from PU-PP

Parameter	
Working capital percentage (% per year)	5
Operating charges (% per year)	25
Plant overhead (% per year)	50
Desired rate of return (% per year)	10
Tax rate (% per year)	40
Plant life (years)	20
Economic life of the project (years)	20
Salvage value (Percent of initial capital cost)	20
Depreciation method	Straight line
Project capital escalation (% per year)	5
Products escalation (% per year)	5
Raw material escalation (% per year)	3.5
Operating and maintenance labor escalation (% per year)	3
Utilities escalation (% per year)	3
General and administrative expenses (% per year)	8

Table S21. Material balances and energy use and generation in different sections for the LOUPs production

Section	Category	Item	Flow	
Feedstock pretreatment	Input streams	PU-PP	10,416.67	kg/h
		Water	9,895.83	kg/h
	Output streams	Ground PU-PP	10,416.67	kg/h
		Water	9,895.83	kg/h
	Energy use	Electricity	12.78	GJ/h
LOUPs production	Input streams	Ground PU-PP	10,416.67	kg/h
		Hydrogen make-up	96.50	kg/h
		Hydrogen recycled	5.52	kg/h
		Pt/STO catalyst	104.17	kg/h
	Output streams	Gaseous product	1,512.94	kg/h
		LOUPs	9,004.84	kg/h
		Pt/STO catalyst recovered	105.06	kg/h
	Energy use	Natural gas	27.06	GJ/h
		Electricity	0.05	GJ/h
Hydrogen recovery	Input streams	Gaseous products	1,512.94	kg/h
	Output streams	Off-gas	1,506.14	kg/h
		Methane	1.29	kg/h
		Recovered hydrogen	5.52	kg/h
	Energy use	Natural gas	0.04	GJ/h
		Electricity	0.21	GJ/h
Heat and power generation	Input streams	Off-gas	1,506.14	kg/h
		Methane	1.29	kg/h
		Air	50,000.00	kg/h
		Water	8,000.00	kg/h
	Output streams	Flue gas	51,507.42	kg/h
		Steam	8,000.00	kg/h
	Energy use	Natural gas	1.27	GJ/h
		Electricity	19.80	GJ/h
	Energy generation	Electricity	43.19	GJ/h

Table S22. Operation specifications for key downstream process units for LOUPs production

Section	Equipment	Item	Value
Feedstock pretreatment	Tank	Outlet pressure (bar) Outlet Temperature (°C)	1.01 62
	Dryer	Outlet pressure (bar) Temperature (°C)	1.01 66
	Grinder	Outlet pressure (bar) Temperature (°C)	1.01 25
LOUPs production	Reactor	Outlet pressure (bar) Temperature (°C)	14.8 310
	Filter	Outlet pressure (bar) Temperature (°C)	1.01 25
Hydrogen recovery	Compressor 1	Discharge pressure (bar) Isentropic efficiency Outlet temperature (°C)	9.8 0.85 94.48
	Flash separator Heater 1	Outlet flash pressure (bar) Temperature (°C)	9.8 26
	PSA	Outlet pressure (bar) Temperature (°C)	9.6 26
Heat and power generation	Compressor 2	Specified discharge pressure (bar) Isentropic efficiency Outlet temperature (°C)	112 0.85 104.99
	MCompressor	Number of stages Outlet pressure (bar)	4 17.71
	Turbine 2	Specified discharge pressure (bar) Isentropic efficiency Outlet temperature (°C)	1.01 0.85 579
	Turbine 3	Specified discharge pressure (bar) Isentropic efficiency Outlet temperature (°C)	1.01 0.85 100
	Pump	Specified discharge pressure (bar) Pump efficiencies	30 0.78
	Steam generator	Inlet hot stream temperature (°C) Inlet hot stream pressure (bar) Outlet hot stream temperature (°C) Outlet hot stream pressure (bar) Inlet cold stream temperature (°C) Inlet cold stream pressure (bar)	579 1.01 150 1.01 25.89 30

Table S23. Main equipment cost used for producing LOUPs from the PU-PP

Section	Main equipment	Installed cost	Source
Feedstock pretreatment	Tank	$537,000	Turton et al.[20]
	Separator	$869,400	APEA[19]
	Dryer	$3,216,000	Turton et al.[20]
	Cooler	$100,900	APEA[19]
	Grinder	$627,900	APEA[19]
	Hopper	$137,603	Connair group[25]
	Conveyor	$1,674,039	Gracida-Alvarez et al.[26]
LOUPs production	Reactor	$5,146,773	APEA[19] and Turton et al.[20]
	Cooler-1	$86,000	APEA[19]
	Cooler-2	$106,600	APEA[19]
	Filter	$849,983	GEA[27]
Hydrogen recovery	Compressor 1	$978,300	APEA[19]
	Cooler3	$74,900	APEA[19]
	Cooler 4	$123,600	APEA[19]
	Flash separator	$142,400	APEA[19]
	Heater 1	$69,100	APEA[19]
	PSA	$3,948,131	Mivechian and Pakizeh[28]
	Compressor 5	$1,279,500	APEA[19]
	Heater 3	$56,000	APEA[19]
Heat and power generation	Heater 2	$67,700	APEA[19]
	Compressor 2	$1,258,500	APEA[19]
	Compressor 3	$7,500,100	APEA[19]
	Combustion reactor	$3,250,000	Turton et al.[20]
	Turbine 2	$7,303,800	APEA[19]
	Steam generator	$275,200	APEA[19]
	Turbine 3	$398,000	APEA[19]
	Pump	$86,800	APEA[19]

APEA: Aspen process economic analyzer v12.

Table S24. Summary of the economic analysis of LOUPs production

Investment Analysis	
Total capital cost ($)	$75,854,445
Total operating cost* ($/yr)	$47,373,674
Total raw materials cost ($/yr)	$33,733,200
Co-product credits ($/yr)	$8,187,598
Total utilities cost ($/yr)	$6,596,610
Desired rate of return (%/yr)	10
Lube oil flow rate (kg/h)	9004
Total catalyst cost($/yr)	1,052,500

*The total operating cost includes the catalyst cost.

Table S25. Comparison of the MSP ($/gal) of Group I, II and III base oils from this study with values reported in the literature

Base oil	This study	Reported values	Reference
Group I	2.59	3.18-3.39	LubesNgreases[29]
Group II	4.27	3.07-4.93	LubesNgreases[29]
Group III	5.66	4.36-5.33	LubesNgreases[29]

Table S26. Comparison of the molecular weight (g/mol) of Group I, II and III base oils from this study with values reported in the literature

Base oil	This study	Reported values	Source
Group I	335	280-390	API[30]
Group II	428	440	API[30]
Group III	423	435	Hackler et al.[31]

API: American Petroleum Institute

Table S27. Comparison of the density (kg/m^3) of Group I, II, and III base oils from this study with values reported in the literature

Base oil	This study	Reported values	Source
Group I	928	700-950	Neste[32]
Group II	938		
Group III	936		

LOUPs analysis data

Table S28. Distribution of the total installed capital cost in different sections for LOUPs production

Process section	Percentage (%)
PU-PP pretreatment	17.83
LOUPs production	15.41
Hydrogen recovery and gas separation	16.61
Heat and power generation	50.14

Table S29. Distribution of the total operating cost (OpEx) among the cost components

Item	Percentage (%)
Raw materials	71.2
Utility	12.8
Catalyst	2.2
Other OpEx	13.8

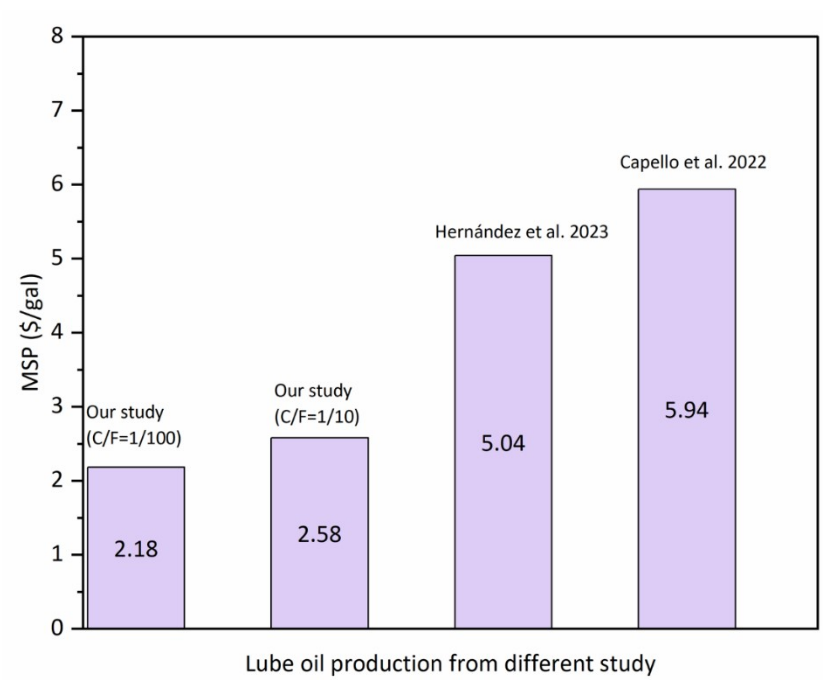

Figure S4. Comparison of the MSP of LOUPs with the referenced resources.[33,34]

Table S30a. Single-point sensitivity analyses for relative change to process variables on the MSP of LOUPs (base case MSP = $2.18/gal)

Process variables	High value (+)	Low value (−)
Catalyst lifetime (yr) (3/ 2 / 1)	−0.67%	2.02%
Catalyst cost (+50%/ BL / −50%)	1.01%	−1.01%
Hydrogen cost (+50% / BL / −50%)	1.80%	−1.80%
Plant life (yr) (40/ BL)	−1.00%	N.A.
Plant size (+50% / BL / −50%)	−13.71%	9.93%
CapEX cost (+50% / BL / −50%)	12.40%	−12.40%
PU-PP cost (+50% / BL / −50%)	33.07%	−33.07%
OpEX (+50% / BL / −50%)	45.46%	−45.46%

CapEx; capital costs, OpEx: Operating costs, BL: Baseline case, N.A.: Not applicable

Table S30b. Sensitivity analysis assuming a % change in the PU-PP to LOUPs conversion (LOUPs yield), co-product credits (i.e., electricity credits), the utility cost reduction for steam production, on some expensive equipment costs, and a financial variable

Process variables	High value (+)	Low value (−)
Steam credits (BL/ −30%)	N.A.	0.50%
Dryer cost (+50% / BL / −50%)	1.00%	−1.00%
COMR cost (+50% / BL / −50%)	1.00%	−1.00%
Filter cost (+50% / BL / −50%)	0.10%	−0.10%
PSA cost (+50% / BL / −50%)	1.00%	−1.00%
Reactor cost (+50% / BL / −50%)	1.00%	−1.00%
No steam credits	2.00%	N.A.
Electricity unit cost (+30% / BL / −30%)	−4.70%	4.70%
Electricity credits (BL /−30%)	N.A.	4.70%
DROR (%) (20 / BL / 7)	28.50%	−5.60%
LOUPs yield (%) (90/ 86 / 60)	−3.90%	44%

BL: Baseline case, N.A.: Not applicable

Table S31. A multivariate sensitivity analysis for the effect of the variation of catalyst cost and catalyst to feedstock ratio (C/F) on MSP of LOUPs. The base case values for C/F ratio and catalyst cost were 1/100 and $842/kg, respectively.

C/F ratio	Catalyst price ($/kg)	MSP ($/gal)
0.01	210.00	2.15
0.01	421.00	2.16
0.01	631.50	2.17
0.01	842.00	2.18
0.01	1,052.00	2.20
0.01	1,263.00	2.21
0.01	1,473.00	2.22
0.01	1,684.00	2.23
0.02	210.00	2.16
0.02	421.00	2.18
0.02	631.50	2.21
0.02	842.00	2.23
0.02	1,052.00	2.25
0.02	1,263.00	2.27
0.02	1,473.00	2.29
0.02	1,684.00	2.32
0.05	210.00	2.20
0.05	421.00	2.25
0.05	631.50	2.31
0.05	842.00	2.36
0.05	1,052.00	2.42
0.05	1,263.00	2.47
0.05	1,473.00	2.53
0.05	1,684.00	2.58
0.1	210.00	2.25
0.1	421.00	2.36
0.1	631.50	2.47
0.1	842.00	2.58
0.1	1,052.00	2.69
0.1	1,263.00	2.80
0.1	1,473.00	2.91
0.1	1,684.00	3.02

Section S4: Life-cycle assessment of conventional base oils refining

The system boundaries for the refining of Group I, II, and III base oils are illustrated in Figure S5, Figure S6, and Figure S7, respectively. These boundaries incorporate the various process stages involved in refining each type of base oil. The pre-flash, atmospheric distillation, vacuum distillation, and deasphalting stages are common to all three base oils. However, solvent extraction and dewaxing are specific to the production of Group I base oil, while hydrotreatment and hydrocracking are exclusive to the refining of Group II and Group III base oils, respectively. To account for the different coproducts generated at various stages, two allocation methods were applied in the analysis. Energy allocation was used to distribute the environmental burdens in the pre-flash, atmospheric distillation, and vacuum distillation stages, as the products from these stages are primarily used as energy products or fuels. Conversely, mass allocation was applied to the remaining stages, where the coproducts are predominantly used as chemicals. This distinction is also indicated in Figure S5, Figure S6, and Figure S7.

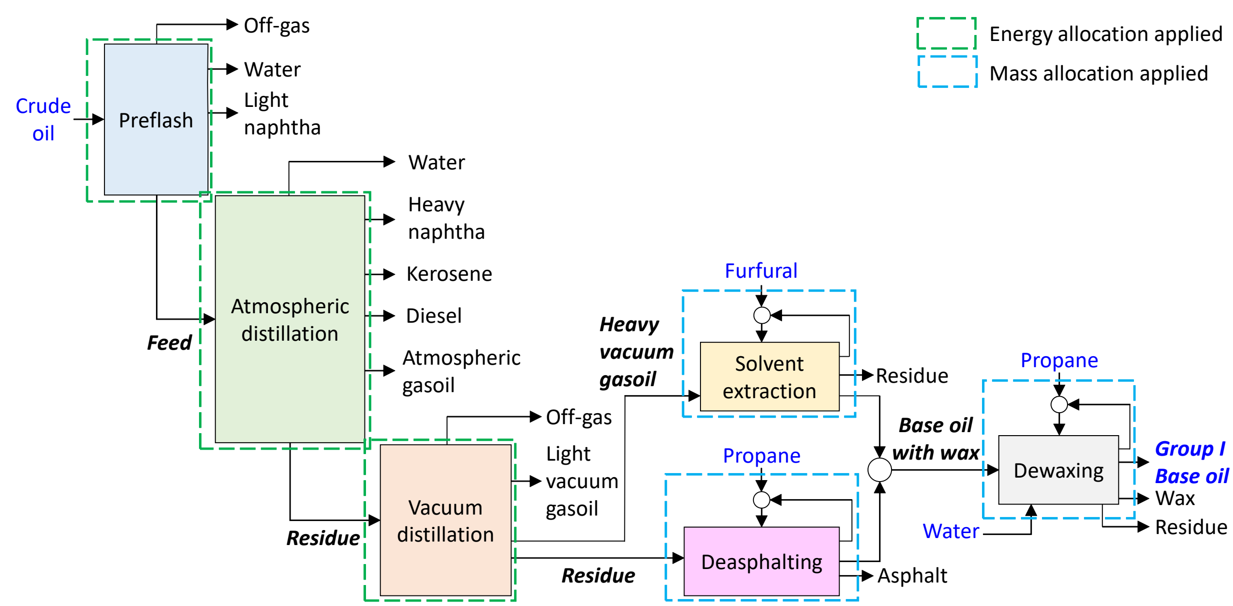

Figure S5. Process pathway for the refining of Group I base oil from crude oil. Stages enclosed by green or blue dashed squares indicate the use of energy-based or mass-based allocation, respectively, to distribute the environmental impacts among coproducts.

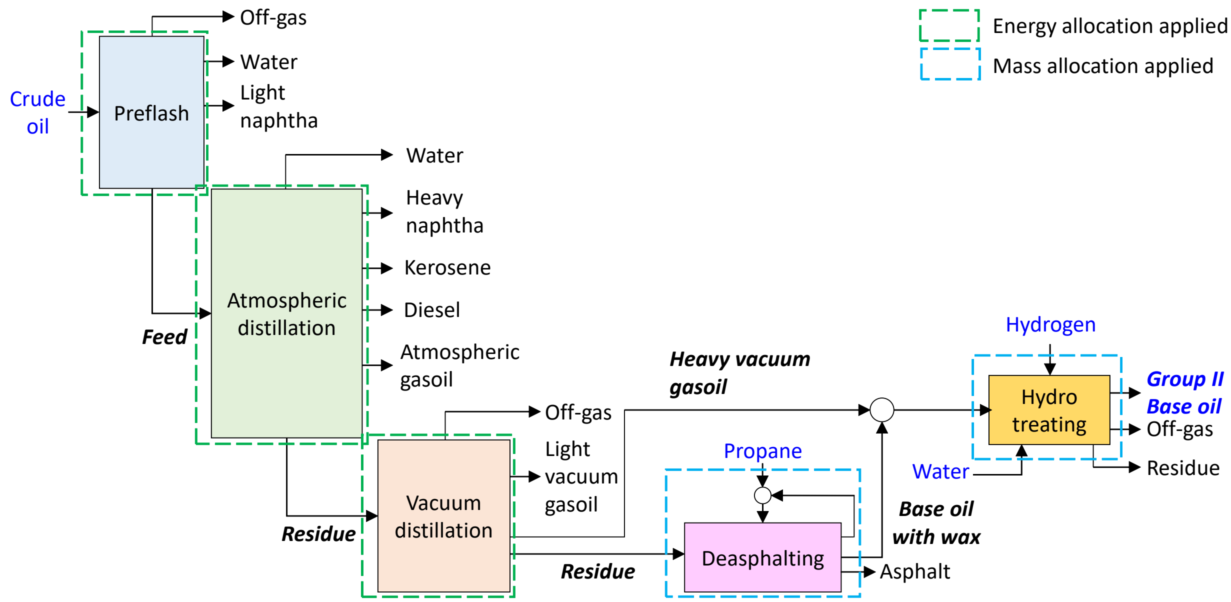

Figure S6. Process pathway for the refining of Group II base oil from crude oil. Stages enclosed by green or blue dashed squares indicate the use of energy-based or mass-based allocation, respectively, to distribute the environmental impacts among coproducts.

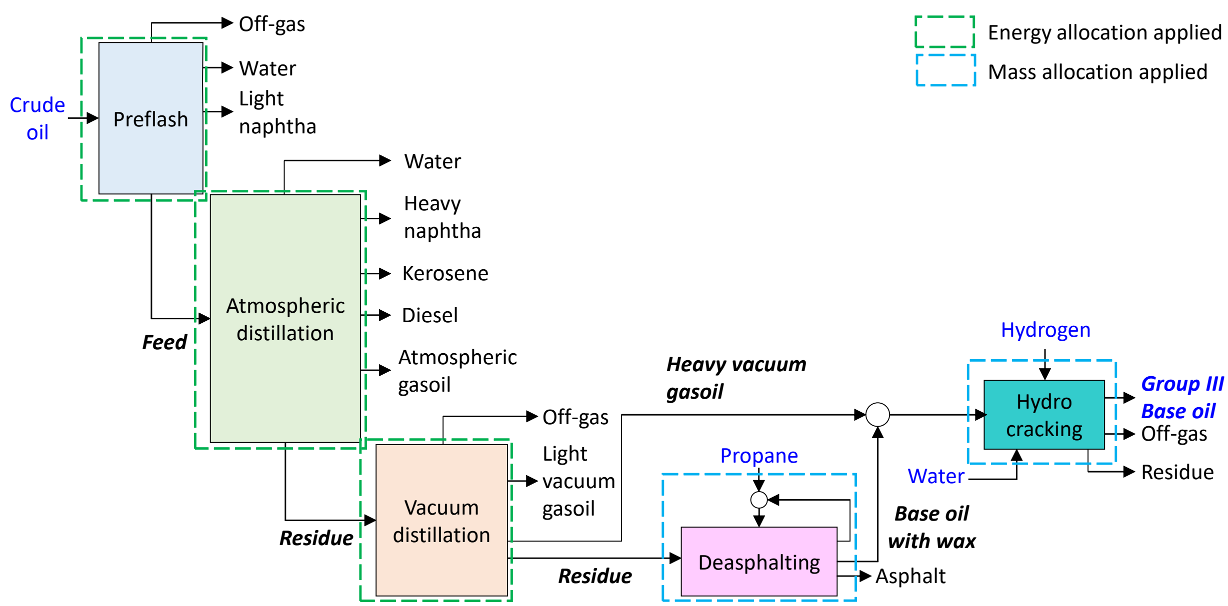

Figure S7. Process pathway for the refining of Group III base oil from crude oil. Stages enclosed by green or blue dashed squares indicate the use of energy-based or mass-based allocation, respectively, to distribute the environmental impacts among coproducts.

The allocation factors for each coproduct generated at each stage of refining for Group I, II, and III base oils are presented in Table S32, Table S33, and Table S34, respectively. As shown in the tables, water and off-gas were excluded from the allocation process. Water, which could be recycled, is not sold as an external coproduct, whereas off-gas is treated as a residue that is combusted before being released into the atmosphere.

Table S32. Allocation factors per stage for the refining of Group I base oils.

Stage	Type of allocation	Coproduct	Allocation factor
Preflash	Energy	Light naphtha	0.156
		Atmospheric Column Feed	0.844
Atmospheric distillation	Energy	Heavy naphtha	0.101
		Kerosene	0.068
		Diesel	0.203
		Atmospheric gasoil	0.053
		Atmospheric residue	0.574
Vacuum distillation	Energy	Light vacuum gasoil	0.087
		Heavy vacuum gasoil	0.187
		Vacuum residue	0.726
Solvent extraction	Mass	Group I Base oil with wax	1.000
Deasphalting	Mass	Group I Base oil with wax	0.819
		Asphalt	0.181
Dewaxing	Mass	Wax	0.001
		GI Base oil	0.999

Table S33. Allocation factors per stage for the refining of Group II base oils.

Stage	Type of allocation	Coproduct	Allocation factor
Preflash	Energy	Light naphtha	0.156
		Atmospheric Column Feed	0.844
Atmospheric distillation	Energy	Heavy naphtha	0.095
		Kerosene	0.138
		Diesel	0.143
		Atmospheric gasoil	0.107
		Atmospheric residue	0.517
Vacuum distillation	Energy	Light vacuum gasoil	0.201
		Heavy vacuum gasoil	0.432
		Vacuum residue	0.368
Deasphalting	Mass	Base oil with wax	0.001
		Asphalt	0.999
Hydrotreatment	Mass	Group II Base oil	1.000

Table S34. Allocation factors per stage for the refining of Group III base oils.

Stage	Type of allocation	Coproduct	Allocation factor
Preflash	Energy	Light naphtha Atmospheric Column Feed	0.159 0.841
Atmospheric distillation	Energy	Heavy naphtha Kerosene Diesel Atmospheric gasoil Atmospheric residue	0.092 0.139 0.144 0.107 0.519
Vacuum distillation	Energy	Light vacuum gasoil Heavy vacuum gasoil Vacuum residue	0.201 0.431 0.368
Deasphalting	Mass	Base oil with wax Asphalt	0.002 0.998
Hydrotreatment	Mass	Group III Base oil	1.000

To develop the life cycle inventory (LCI) data for each stage of base oil production, the quantities of material and energy inputs used in that stage were divided by the coproduct of interest and then multiplied by the corresponding allocation factor for that coproduct at that stage. Using this methodology, the LCI data, after allocation, were compiled for each type of base oil. This information is presented in Table S35, Table S36, and Table S37 for Group I, II, and III base oils, respectively. The aggregated life cycle inventory for each base oil, derived from this data, is shown in Table 1 of the main manuscript.

Table S35. Life cycle inventory data per stage (after allocation) for the refining of Group I base oils.

Stage	Input category	Input type	Value
Preflash	Material (MJ/kg atmospheric column feed)	Crude oil	43.22
	Energy (MJ/kg atmospheric column feed)	Natural gas	0.45
Atmospheric distillation	Material (kg/kg atmospheric residue)	Atmospheric column feed	0.98
	Energy (MJ/kg atmospheric residue)	Natural gas	0.49
Vacuum distillation	Material (kg/kg heavy vacuum gasoil)	Atmospheric residue	1.03
	Energy (MJ/kg heavy vacuum gasoil)	Natural gas	0.09
	Material (kg/kg vacuum residue)	Atmospheric residue	0.99
	Energy (MJ/kg vacuum residue)	Natural gas	0.10
Solvent extraction	Material (kg/kg base oil with wax)	Heavy vacuum gasoil Furfural	1.02 0.006
	Energy (MJ/kg base oil with wax)	Natural gas Electricity	2.39 0.002
Deasphalting	Material (kg/kg base oil with wax)	Vacuum residue Propane	0.96 0.04
	Energy (MJ/kg base oil with wax)	Natural gas Electricity	0.07 0.01
Dewaxing	Material (kg/kg Group I base oil)	Base oil with wax from heavy vacuum gasoil Base oil with wax from vacuum residue Propane	0.22 0.77 0.01
	Energy (MJ/kg Group I base oil)	Natural gas Electricity	0.57 0.11

Table S36. Life cycle inventory data per stage (after allocation) for the refining of Group II base oils.

Stage	Input category	Input type	Value
Preflash	Material (MJ/kg atmospheric column feed)	Crude oil	43.47
	Energy (MJ/kg atmospheric column feed)	Natural gas	0.46
Atmospheric distillation	Material (kg/kg atmospheric residue)	Atmospheric column feed	0.98
	Energy (MJ/kg atmospheric residue)	Natural gas	0.57
Vacuum distillation	Material (kg/kg heavy vacuum gasoil)	Atmospheric residue	1.01
	Energy (MJ/kg heavy vacuum gasoil)	Natural gas	0.62
	Material (kg/kg vacuum residue)	Atmospheric residue	0.98
	Energy (MJ/kg vacuum residue)	Natural gas	0.59
Deasphalting	Material (kg/kg base oil with wax)	Vacuum residue Propane	0.98 0.02
	Energy (MJ/kg base oil with wax)	Natural gas Electricity	0.10 0.01
Hydrotreatment	Material (kg/kg Group II base oil)	Heavy vacuum gasoil Base oil with wax from vacuum residue	1.03 0.001
	Material (MJ/kg Group II base oil)	Hydrogen make-up	3.77
	Energy (MJ/kg Group II base oil)	Natural gas Electricity	4.45 4.43

Table S37. Life cycle inventory data per stage (after allocation) for the refining of Group III base oils.

Stage	Input category	Input type	Value
Preflash	Material (MJ/kg atmospheric column feed)	Crude oil	43.45
	Energy (MJ/kg atmospheric column feed)	Natural gas	0.46
Atmospheric distillation	Material (kg/kg atmospheric residue)	Atmospheric column feed	0.98
	Energy (MJ/kg atmospheric residue)	Natural gas	0.57
Vacuum distillation	Material (kg/kg heavy vacuum gasoil)	Atmospheric residue	1.01
	Energy (MJ/kg heavy vacuum gasoil)	Natural gas	0.62
	Material (kg/kg vacuum residue)	Atmospheric residue	0.98
	Energy (MJ/kg vacuum residue)	Natural gas	0.59
Deasphalting	Material (kg/kg base oil with wax)	Vacuum residue Propane	0.99 0.006
	Energy (MJ/kg base oil with wax)	Natural gas Electricity	2.93 0.02
Hydrocracking	Material (kg/kg Group II base oil)	Heavy vacuum gasoil Base oil with wax from vacuum residue	1.00 0.002
	Material (MJ/kg Group II base oil)	Hydrogen make-up	4.66
	Energy (MJ/kg Group II base oil)	Natural gas Electricity	8.76 7.47

Section S5. Life cycle assessment of conventional end-of-life (EOL) management of PU-PP

This study also compares the conversion of post-use (PU-PP) to lubricating oils form upcycled plastics (LOUPs) with conventional end-of-life (EOL) management technologies. The hydrogenolysis process is designed to handle PU-PP that is not currently subjected to mechanical recycling. Consequently, the comparison with conventional EOL management focused exclusively on current practices for handling non-recycled plastics. Due to a lack of specific information on PU-PP film from material recovery facilities (MRFs), general data for the waste management of plastics in the United States was utilized in this study.

The system boundary for the conventional EOL management of PU-PP film is shown in Figure S8. The LCA was conducted using a functional unit of one kg of PU-PP. The process starts with the curbside collection of PU-PP using a refuse truck with a payload capacity of 11.8 tonnes, covering a distance of 80.5 km.[35,36] Afterward, PU-PP is sorted from other types of waste in a MRF that utilizes 4.7 kWh of electricity and 0.7 L of diesel per tonne of PU-PP processed.[37] Approximately 23% of the PU-PP is lost during the sorting process.[37] After sortation, PU-PP that is not recycled is transported to a landfill for permanent storage or incineration. Information from the U.S. EPA[38] establishes that 80% of the non-recycled material is stored in landfills, while the remaining 20% is incinerated. The transportation to landfill is carried out using a medium-heavy-duty truck with a capacity of 20 tonnes, covering a distance of 40 km.[36,39] The emissions from the incineration of PU-PP were estimated based on the assumption that all carbon in the material is fully converted to CO_2. This study considered a carbon content for PU-PP of 86%.[40] During incineration, the energy released from PU-PP combustion can be utilized for electricity generation. Therefore, two scenarios were analyzed: one where electricity is not produced (“without energy recovery” scenario) and another where electricity is generated from incineration, (“with energy recovery” scenario). The amount of energy produced during incineration was estimated at 2.94 kWh per kg of PU-PP, based on the lower heating value of PP (42.43 MJ/kg)[41] and a power generation efficiency of 25%. The electricity generated is assumed to displace electricity from the average U.S. grid and therefore a greenhouse gas (GHG) emissions credit of 0.44 kg CO_2e/kWh is included in the estimations.

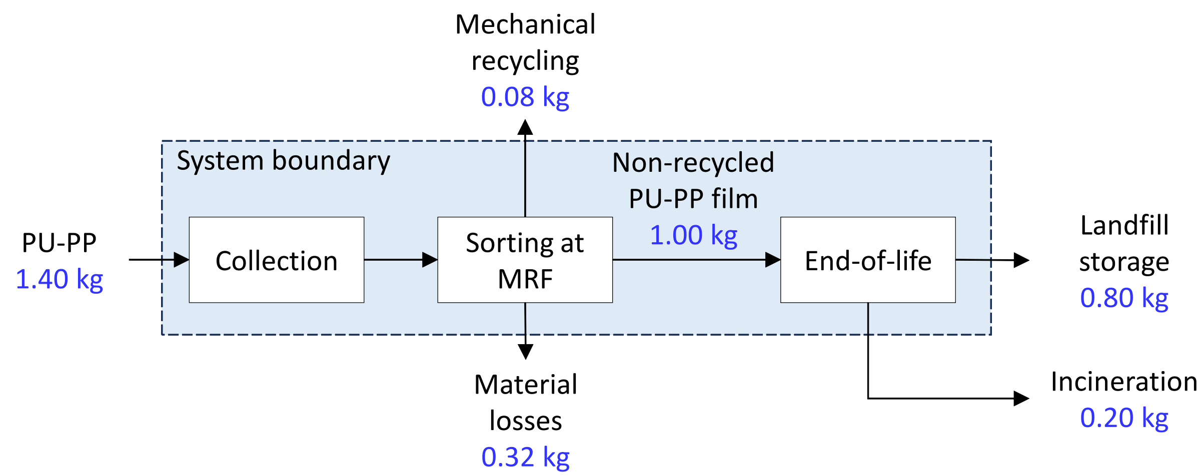

Figure S8. System boundary for the conventional EOL management of PU-PP

The GHG emissions for the scenarios of incineration with and without energy recovery are shown in Figure S9a. Without energy recovery, the GHG emissions are 0.7 kg CO_2e/kg PU-PP, whereas with energy recovery, the GHG emissions are lowered to 0.4 kg CO_2e/kg PU-PP, representing a 39% reduction compared to the scenario without energy recovery. The emissions from the incineration process itself are estimated at 0.6 kg CO_2e/kg PU-PP, while the GHG emission credits from energy recovery are estimated at 0.3 kg CO_2e/kg PU-PP. Most of the emissions are attributed to the incineration process, with only 5% attributed to transportation, collection, and sorting in both scenarios. The fossil energy use for conventional waste management was estimated at 0.5 MJ/kg PU-PP for incineration without energy recovery and −3.7 MJ/kg PU-PP for incineration with energy recovery (see Figure S9b). Among the processing stages, collection was the largest contributor to fossil energy use, accounting for 79% of the total fossil energy consumption. This is primarily due to the diesel used in refuse trucks for collection. In the case of energy recovery, the credits from avoided fossil energy (4.2 MJ/kg PU-PP) exceeded the process-related fossil energy consumption (0.5 MJ/kg PU-PP), resulting in the observed negative fossil energy use. As observed in Figure S9c, water consumption for conventional waste management without energy recovery was estimated to be close to zero L/kg PU-PP, with credits of 1.3 L/kg PU-PP observed in the energy recovery scenario. This significant amount of avoided water consumption is consistent with the water consumption associated with electricity generation, which is estimated at 0.6 L per MJ of electricity.

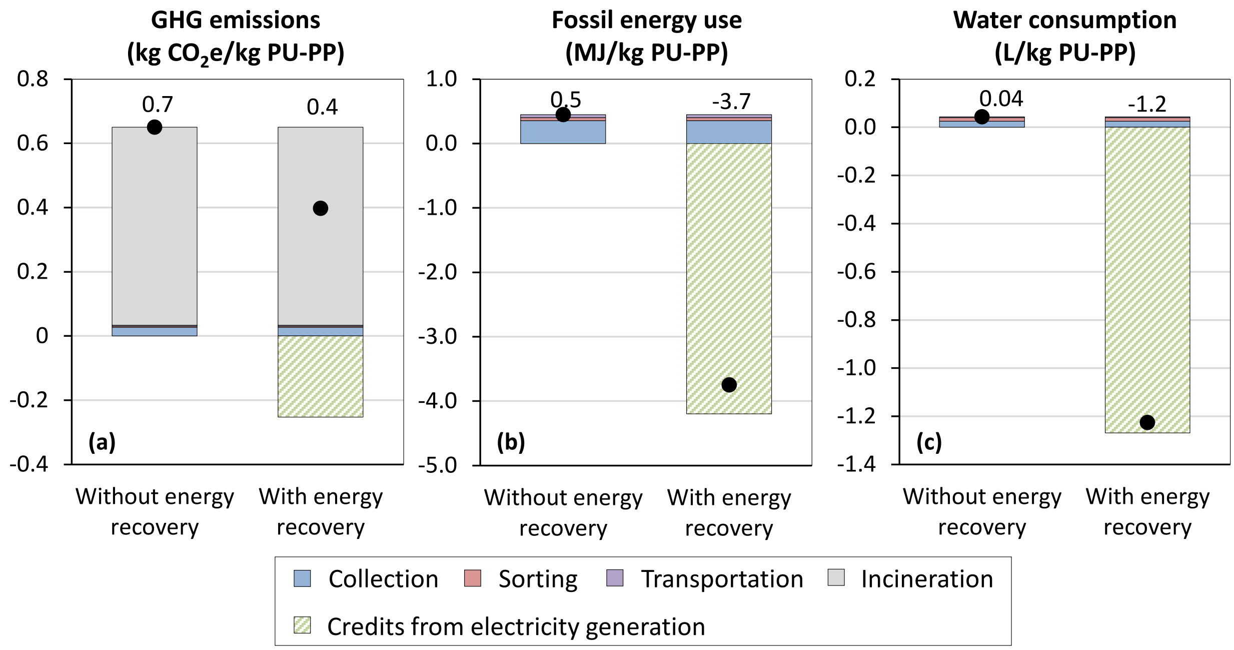

Figure S9. Environmental impacts of conventional EOL management of PU-PP: (a) GHG emissions, (b) fossil energy use, and (c) water consumption. The black dots represent net GHG emissions, fossil energy use, and water consumption.

Section S6. Supplementary information for the life cycle assessment of LOUPs

S6.1 Counterfactual scenario

Figure S10b illustrates the counterfactual scenario to produce LOUPs. In this scenario, the emissions associated with the conventional EOL management of PU-PP film are avoided. Specifically, for each kilogram of PU-PP film converted into LOUPs, the emissions from the landfill storage of 0.8 kg and the incineration of 0.2 kg of PU-PP film are avoided. Consequently, a credit can be subtracted from the total process-related GHG emissions of the hydrogenation process. The inclusion of this credit into the GHG emissions estimations is discussed in the "GHG emissions of the production of LOUPs" of the main manuscript.

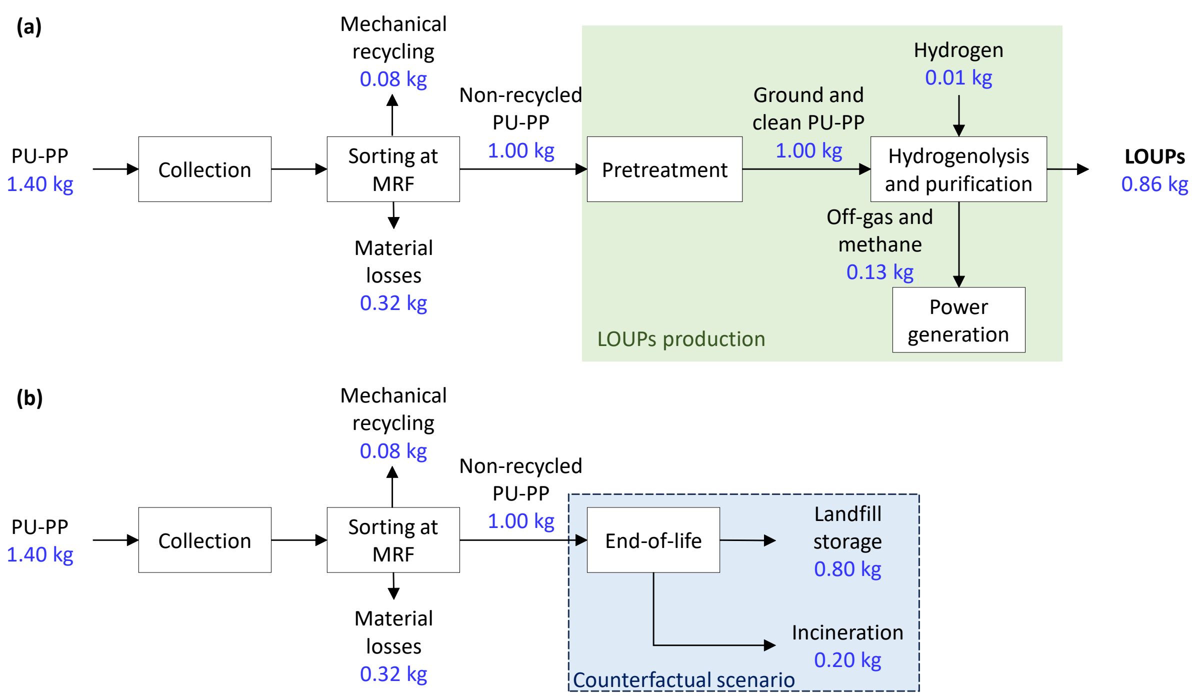

Figure S10. Block diagrams for (a) Conversion of PU-PP to LOUPs via hydrogenolysis and (b) avoided conventional EOL management of PU-PP (counterfactual scenario).

S6.2 Fossil energy use and water consumption of the production of LOUPs

Figure S11a and Figure S11b present the fossil energy use and water consumption, respectively, of the production of LOUPs under different co-product treatment methods. These results are further discussed in the "Fossil energy use and water consumption of the production of LOUPs" section of the main manuscript.

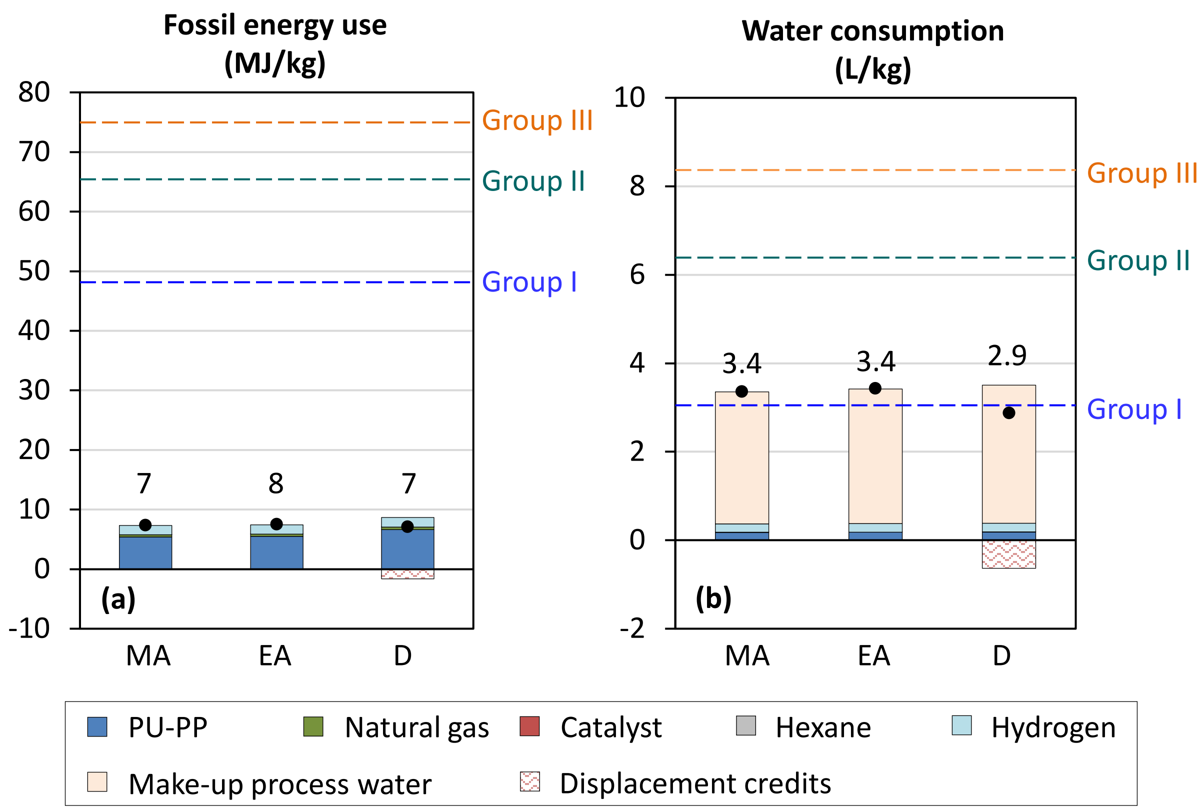

Figure S11. (a) Fossil energy use and (b) water consumption of the production of LOUPs. Dashed lines indicate the impacts of conventional base oil production from crude oil. The black dots represent net fossil energy use and water consumption. MA: Market-based allocation, EA: Energy-based allocation, D: Displacement.

S6.3 GHG emissions, fossil energy use, and water consumption of the treatment of PU-PP through hydrogenolysis

A displacement method was utilized for the LCA with a functional unit of one kg of processed PU-PP. In this method, all the environmental impacts associated with the conversion process are allocated to the feedstock, with the credits of the electricity generated and sold to the grid subtracted from the overall impact.

The GHG emissions associated with the hydrogenolysis of PU-PP are presented in Figure S12a. The process-related GHG emissions are estimated at 0.6 kg CO_2e/kg PU-PP, from which the credits for displaced coproducts are subtracted. The credits for the displacement of grid electricity are estimated at 0.1 kg CO_2e/kg PU-PP, while the displacement credits associated with the production of LOUPs vary depending on the type of base oil being displaced. The analysis indicates that the displacement credits are estimated at 0.4, 1.4, and 2.0 kg CO_2e/kg PU-PP for Group I, Group II, and Group III base oils, respectively. As a result, the net GHG emissions of the hydrogenolysis process range between 0.08 and −1.50 kg CO_2e/kg PU-PP, which are lower than those associated with the conventional EOL management of PU-PP with energy recovery (see Figure S9a). The estimated reductions in GHG emissions from transitioning from conventional EOL management to hydrogenolysis range between 0.3 and 2.2 kg CO_2e/kg PU-PP.

The GHG emissions reported for hydrogenolysis in this study are slightly lower than those reported by Hernandez et al.,[33] who estimated 0.1 kg CO_2e/kg LDPE. The authors considered the displacement of base oil (Group III) and fuels, while for the present study only electricity and base oils are subtracted from the hydrogenolysis GHG emissions. However, it is important to note that our results vary significantly depending on the base oil displaced, as the GHG emissions estimates in this study are distinct to each base oil type, unlike previous studies.

Comparisons of fossil energy use and water consumption between hydrogenolysis and conventional EOL management of PU-PP are shown in Figures S12b and S12c, respectively. Similar to GHG emissions, the fossil energy use in hydrogenolysis is lower than that of conventional EOL management. The fossil energy use of hydrogenolysis ranges from −36 to −59 MJ/kg PU-PP, depending on the type of conventional base oil being displaced. These values are significantly lower than those observed for conventional EOL management with energy recovery of PU-PP. Water consumption for hydrogenolysis ranges between −0.1 and −4.7 L/kg PU-PP, which is lower than the water consumption observed in conventional EOL management without energy recovery. However, when Group I base oil is displaced by LOUPs, the water consumption is higher compared to conventional EOL management with energy recovery. This is due to the combined effect of the water consumption avoided through conventional EOL management with energy recovery and the lower water consumption displaced from Group I base oil. Based on these findings, hydrogenolysis demonstrates reduced environmental impacts compared to conventional EOL management in terms of GHG emissions and fossil energy use. However, for water consumption, the outcome could be improved by implementing water treatment and recycling processes.

Additional benefits of hydrogenolysis over conventional EOL treatment include the reduction of solid waste generation and an increase in the recyclability of materials. Analyzing the supply chain from PU-PP collection to hydrogenolysis (Figure S10a), producing one kilogram of LOUPs through hydrogenolysis avoids the generation of ~1.2 kg of solid waste. This represents a 100% reduction in the solid waste generation of non-recycled PU-PP, which would otherwise be disposed of through landfill or incineration in conventional waste management. Furthermore, hydrogenolysis converts PU-PP into LOUPs at a yield of 86%, increasing the amount of PU-PP that is reused compared to conventional EOL management.

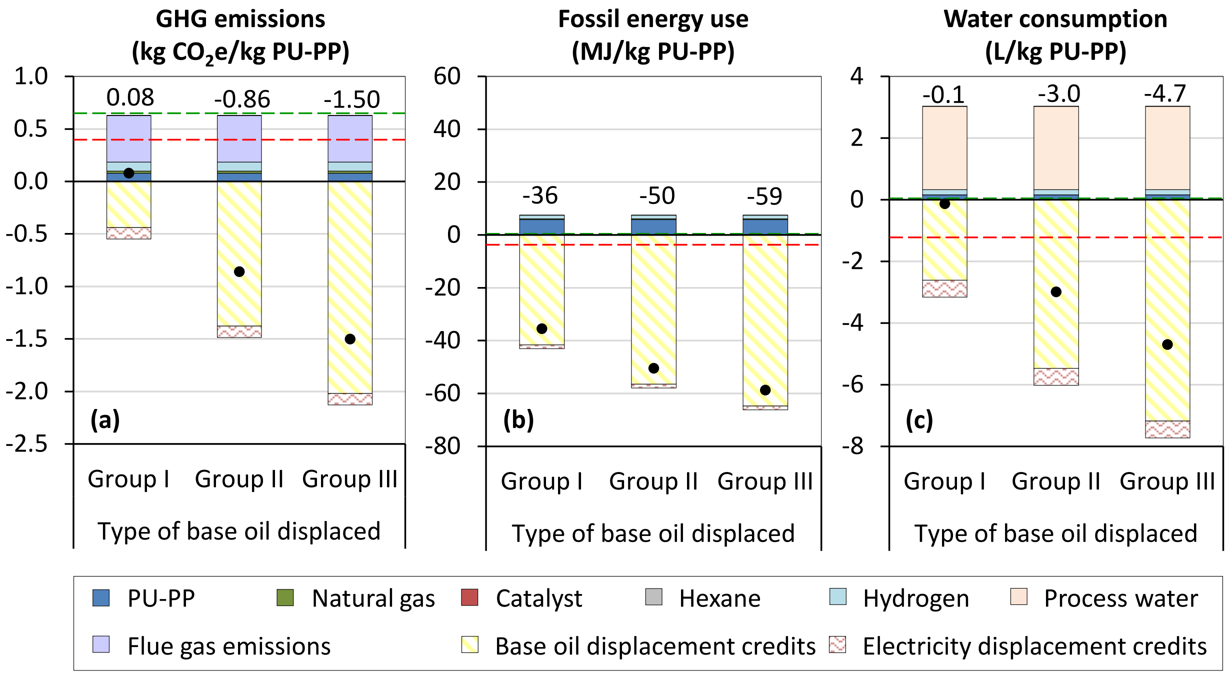

Figure S12. (a) GHG emissions, (b) Fossil energy use, and (c) water consumption associated with the processing of one kg of PU-PP through hydrogenolysis under the displacement of different types of conventional base oils. Black dots represent net GHG emissions, fossil energy use, and water consumption. The green and red dashed lines represent the impacts of conventional EOL management without and with energy recovery, respectively.

References

1 M. T. Fouladvand, J. Asadi and M. N. Lotfollahi, *Chemical Engineering Research and Design*, 2021, **165**, 118–128.
2 J. J. Espada, B. Coto, R. van Grieken and J. M. Moreno, *Chemical Engineering and Processing: Process Intensification*, 2008, **47**, 1398–1403.
3 S. M. Fakhr Hoseini, M. S. Hatamipour, T. Tavakkoli and A. Montahaee, *Ind. Eng. Chem. Res.*, 2009, **48**, 9325–9330.
4 Solvent dewaxing, Solvent Dewaxing |Petroleum Refining, https://courses.ems.psu.edu/fsc432/content/solvent-dewaxing, (accessed 1 December 2023).
5 S. Ahn, S. Shin, S. I. Im, K. B. Lee and N. S. Nho, *Korean J. Chem. Eng.*, 2016, **33**, 265–270.
6 J. H. Gary, G. E. Handwerk and M. J. Kaiser, *Petroleum Refining. Technology and Economics.*, CRC Press, Boca Raton, FL, 5th., 2007.
7 AspenTech, Getting started modeling petroleum processes, https://inside.mines.edu/~jjechura/Refining/AspenPlusPetroleumV7_1-Start.pdf.
8 U.S. EIA, U.S. No 2 Diesel Wholesale/Resale Price by Refiners (Dollars per Gallon), https://www.eia.gov/dnav/pet/hist/LeafHandler.ashx?n=PET&s=EMA_EPD2D_PWG_NUS_DPG&f=M, (accessed 1 January 2024).
9 U.S. EIA, U.S. Kerosene Wholesale/Resale Price by Refiners (Dollars per Gallon), https://www.eia.gov/dnav/pet/hist/LeafHandler.ashx?n=PET&s=EMA_EPPK_PWG_NUS_DPG&f=M, (accessed 1 January 2024).
10 U.S. EIA, Today in Energy Daily Prices - U.S. Energy Information Administration (EIA), https://www.eia.gov/todayinenergy/prices.php/propane, (accessed 1 January 2024).
11 Riogen, *Catalyst*, Personal communication, 2023.
12 New York State Department of Transportation, Fuel, asphalt, & steel Price Adjustments, https://www.dot.ny.gov/main/business-center/contractors/construction-division/fuel-asphalt-steel-price-adjustments, (accessed 1 January 2024).
13 Naphtha, Business analytiq, http://lookerstudio.google.com/reporting/0af9924c-0480-40f4-85a3-5fbfc19084ab/page/68C7C?feature=opengraph, (accessed 1 January 2024).
14 Paraffin wax, Business analytiq, http://lookerstudio.google.com/reporting/75b119ad-9d92-4399-b43a-acf8f5bd410f/page/68C7C?feature=opengraph, (accessed 1 January 2024).
15 U.S.EIA, Domestic Crude Oil First Purchase Prices by Area, https://www.eia.gov/dnav/pet/pet_pri_dfp1_k_m.htm.
16 G. H. C. Dubbink, T. R. J. Geverink, B. Haar, H. W. Koets, A. Kumar, H. van den Berg, A. G. J. van der Ham and J.-P. Lange, 2021, **15**, 1021–1030.
17 U.S. EIA, Electricty power monthly. Table 5.3. Average Price of Electricity to Ultimate Customers: Total by End-Use Sector, 2014 - May 2024 (Cents per Kilowatthour), https://www.eia.gov/electricity/monthly/epm_table_grapher.php?t=epmt_5_3, (accessed 1 January 2024).
18 U.S. EIA, U.S. Natural Gas Prices, https://www.eia.gov/dnav/ng/ng_pri_sum_dcu_nus_m.htm, (accessed 1 January 2024).
19 Aspentech, Aspen Process Economic Analyzer, https://www.aspentech.com/en/products/engineering/aspen-process-economic-analyzer, (accessed 1 January 2024).
20 R. Turton, J. Shaeiwitz, D. Bhattacharyya and W. Whiting, *Analysis, Synthesis, and Design of Chemical Processes*, Pearson, Boston, 2018.

21 R. Davis, M. Wiatrowski, C. Kinchin and D. Humbird, *Conceptual Basis and TechnoEconomic Modeling for Integrated Algal Biorefinery Conversion of Microalgae to Fuels and Products 2019 NREL TEA Update: Highlighting Paths to Future Cost Goals via a New Pathway for Combined Algal Processing,* NREL/TP-5100-75168, National Renewable Energy Lab. (NREL), Golden, CO, 2020.
22 Resource Plastics, *Post-use polypropylene*, Personal communication, 2024.
23 Resource Recyling, *Post-use polypropylene*, Personal communication, 2024.
24 ChemCatBio, CatCost v1.1.0 https://catcost.chemcatbio.org, 2021.
25 Conair, *Hopper*, Personal communication, 2024.
26 U. R. Gracida-Alvarez, O. Winjobi, J. C. Sacramento-Rivero and D. R. Shonnard, *ACS Sustainable Chem. Eng.*, 2019, **7**, 18254–18266.
27 GEA, GEA "Plug & Win" Triple win centrifuge skids for craft brewers., https://stiener.es/wp-content/uploads/2019/01/Centr%C3%ADfugas-GEA-Cerveza.pdf, (accessed 30 May 2024).
28 A. Mivechian and M. Pakizeh, *Korean J. Chem. Eng.*, 2013, **30**, 937–948.
29 Lube N Greases, *Base oils*, Personal communication, 2023.
30 API, *Lubricating oil basestocks: American Petroleum Institute (API) Petroleum HPV Testing Group*, 2011.
31 R. A. Hackler, K. Vyavhare, R. M. Kennedy, G. Celik, U. Kanbur, P. J. Griffin, A. D. Sadow, G. Zang, A. Elgowainy, P. Sun, K. R. Poeppelmeier, A. Erdemir and M. Delferro, *ChemSusChem*, 2021, **14**, 4181–4189.
32 Neste, Basic concepts of lubricants, https://web.archive.org/web/20231001132102/https://www.neste.com/products/all-products/fossil-products/lubricants/basic-concepts-lubricants#e8003fc2, (accessed 1 January 2024).
33 B. Hernández, P. Kots, E. Selvam, D. G. Vlachos and M. G. Ierapetritou, *ACS Sustainable Chem. Eng.*, 2023, **11**, 7170–7181.
34 V. Cappello, P. Sun, G. Zang, S. Kumar, R. Hackler, H. E. Delgado, A. Elgowainy, M. Delferro and T. Krause, *Green Chem.*, 2022, **24**, 6306–6318.
35 Argonne National Laboratory, *Research and Development Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model (R&D GREET) ® (2023 Excel)*, 2023.
36 U. R. Gracida-Alvarez, H. Xu, P. T. Benavides, M. Wang and T. R. Hawkins, *ACS Sustainable Chem. Eng.*, 2023, **11**, 514–524.
37 P. N. Pressley, J. W. Levis, A. Damgaard, M. A. Barlaz and J. F. DeCarolis, *Waste Management*, 2015, **35**, 307–317.
38 U.S. EPA, *Advancing Sustainable Materials Management: 2018 Tables and Figures*, 2020.
39 ANL, Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET) Model ® (R&D 2023 Excel), https://doi.org/10.11578/GREET-Excel-2023/dc.20230907.1.
40 U.S. EPA, Plastics, https://archive.epa.gov/epawaste/conserve/tools/warm/pdfs/Plastics.pdf, (accessed 17 July 2022).
41 C. Areeprasert, J. Asingsamanunt, S. Srisawat, J. Kaharn, B. Inseemeesak, P. Phasee, C. Khaobang, W. Siwakosit and C. Chiemchaisri, *Energy Procedia*, 2017, **107**, 222–226.