

Electronic Supplementary Information

Techno-economic analysis and life cycle assessment for catalytic fast pyrolysis of mixed plastic waste

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Lists of abbreviations:

- ACCE: Aspen Capital Cost Estimator
- AWARE: Available WATER REmaining
- BAHX: Brazed Aluminum Heat Exchanger
- BTG-BTL: Biomass Techno
- BTX: Benzene, Toluene, Xylene
- CFP: Catalytic Fast Pyrolysis
- C/F ratio: Catalyst-to-feed ratio
- DMF: Dimethylformamide
- ED: Extractive distillation
- EIA: Environmental Protection Agency
- ESI: Electronic Supplementary Information
- EXP: Expander
- FCC: Fluid Catalytic Cracking
- GHG: Greenhouse Gas
- HC: Hydrocarbon
- HDPE: High-Density Polyethylene
- IRR: Internal Rate of Return
- KO drum: Knock-out drum
- LCA: Life cycle assessment
- LDPE: Low-Density Polyethylene
- LHV: Lower Heating Value
- LLDPE: Linear Low-Density Polyethylene
- MEA: Monoethanolamine
- MFI: Materials Flows Through Industry
- MITA: Minimum Temperature Approach
- MPW: Mixed Plastic Waste
- MRF: Materials Recovery Facility
- MSP: Minimum Selling Price
- MSW: Municipal Solid Waste
- NGLs: Natural Gas Liquids
- NIST-TDE: National Institute of Science and Technology ThermoDataEngine
- NMP: N-formylmorpholine
- NPV: Net Present Value
- NREL – National Renewable Energy Laboratory
- NRTL-RK – Nonrandom Two-Liquid-Redlich-Kwong
- OSBL: Outside Battery Limits
- PET: Poly(ethylene terephthalate)
- PFD: Process Flow Diagram
- PP: Polypropylene
- PS: Polystyrene
- PVC: Poly(vinyl chloride)
- RFO: Renewable Fuel Oil
- RTP: Rapid Thermal Processing
- TEA: Techno-economic Assessment
- TPD: Tonnes Per Day
- TRL: Technology Readiness Level
- TRACI: Tool for the Reduction and Assessment of Chemicals and Other Environmental Impacts
- UNIQUAC: Universal Quasichemical
- USD: United States Dollars
- WTI: West Texas Intermediate

A. Supporting figures

Base case model construction: Process flow diagrams (PFDs)

a. Process area's: Feedstock Pretreatment and Catalytic Fast Pyrolysis

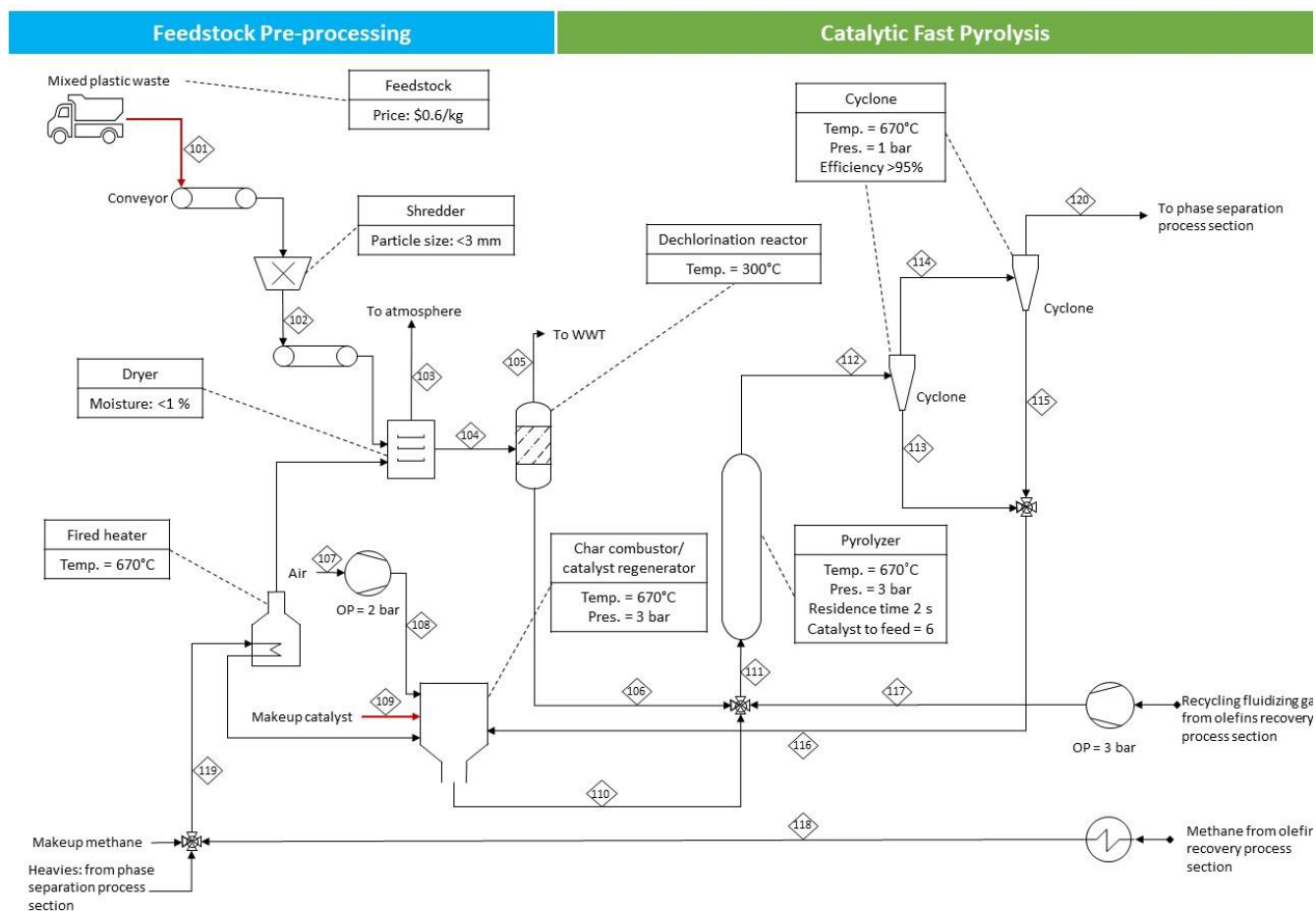


Fig. S1. Detailed PFD of feedstock pre-processing and catalytic fast pyrolysis process sections (base case). Mixed plastic wastes and other raw inputs are shown in red; intermediate, recycle, and waste streams are shown in black.

Streams composition

Components	Units	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120
Total Flow	kg/hr	10000	10000	21315	10000	724	9783	19872	19872	272	58305	75709	75709	296	17401	3	299	7621	223	872	17103
Volume Flow	l/min	186	186	328090	186	2693	323	287183	188813	0.8	159	554103	560992	2	557216	0.02	2.25	15626	1613	12011	475451
Temperature	°C	25	25	50	100	300	301	32.2	123	16	16	670	670	670	670	670	670	670	12	240	670
Pressure	bar	1	1	1	1	1	3	1	2	2	2	3	1	1	1	1	1	3	5	1	1
LDPE	kg/hr	2100	2100	0	2100	0	2100	0	0	0	0	2100	0	0	0	0	0	0	0	0	0
HDPE	kg/hr	1900	1900	0	1900	0	1900	0	0	0	0	1900	0	0	0	0	0	0	0	0	0
PP	kg/hr	2400	2400	0	2400	0	2400	0	0	0	0	2400	0	0	0	0	0	0	0	0	0
PS	kg/hr	1100	1100	0	1100	0	1100	0	0	0	0	1100	0	0	0	0	0	0	0	0	0
LLDPE	kg/hr	1800	1800	0	1800	0	1800	0	0	0	0	1800	0	0	0	0	0	0	0	0	0
PET	kg/hr	300	300	0	300	0	300	0	0	0	0	300	0	0	0	0	0	0	0	0	0
PVC	kg/hr	400	400	0	400	0	8	0	0	0	0	8	0	0	0	0	0	0	0	0	0
Benzene	kg/hr	0	0	0	0	0	163	0	0	0	0	163	0	0	0	0	0	0	0	0	0
Water	kg/hr	0	0	1635	0	507	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HCl	kg/hr	0	0	0	0	217	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Catalyst	kg/hr	0	0	0	0	0	0	0	0	0	58305	58305	58305	0	0	0	0	0	0	0	0
Air	kg/hr	0	0	0	0	0	0	19872	19872	0	0	0	0	0	0	0	0	0	0	0	0
H2	kg/hr	0	0	0	0	0	0	0	0	0	24	38	38	0	14	0	0	24	14	14	38
CH4	kg/hr	0	0	0	0	0	0	0	0	272	259	405	405	0	149	0	0	258	148	146	405
C2H6	kg/hr	0	0	0	0	0	0	0	0	0	158	248	248	0	92	0	0	158	0.02	0.023	248
C3H8	kg/hr	0	0	0	0	0	0	0	0	0	489	778	778	0	294	0	0	489	0	0	778
C2H4	kg/hr	0	0	0	0	0	0	0	0	0	1170	1833	1833	0	674	0	0	1170	22	25	1833
C3H6	kg/hr	0	0	0	0	0	0	0	0	0	2651	4201	4201	0	1579	0	0	2651	0	0	4201
HCl	kg/hr	0	0	0	0	0	0	0	0	0	11	0	0	0	0	0	0	0	0	0	0
C4H10	kg/hr	0	0	0	0	0	0	0	0	0	563	946	946	0	391	0	0	563	0	0	946
N-C6H14	kg/hr	0	0	0	0	0	0	0	0	0	9	31	31	0	23	0	0	9	0	0	31
C7H14	kg/hr	0	0	0	0	0	0	0	0	0	13	121	121	0	110	0	0	13	0	0	121
BENZENE	kg/hr	0	0	0	0	0	0	0	0	0	198	205	205	0	173	0	0	35	0	0	205
TOLUENE	kg/hr	0	0	0	0	0	0	0	0	0	22	654	654	0	644	0	0	22	0	0	654
XYLENE	kg/hr	0	0	0	0	0	0	0	0	0	6	1368	1368	0	1388	0	0	6	0	0	1368
CUMENE	kg/hr	0	0	0	0	0	0	0	0	0	1	1050	1050	0	1068	0	0	1	0	0	1050
N-C8H18	kg/hr	0	0	0	0	0	0	0	0	0	3	240	240	0	241	0	0	3	0	0	240
N-C9H20	kg/hr	0	0	0	0	0	0	0	0	0	0.5	378	378	0	385	0	0	0.47	0	0	378
N-C10H22	kg/hr	0	0	0	0	0	0	0	0	0	0	126	126	0	128	0	0	0	0	0	126
C11H24	kg/hr	0	0	0	0	0	0	0	0	0	0	168	168	0	171	0	0	0	0	0	168
C12H26	kg/hr	0	0	0	0	0	0	0	0	0	0	10	10	0	10	0	0	0	0	0	10
C13H28	kg/hr	0	0	0	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	0	1
C15H32	kg/hr	0	0	0	0	0	0	0	0	0	0	570	570	0	580	0	0	0	0	0	554
C24H50	kg/hr	0	0	0	0	0	0	0	0	0	0	96	96	0	98	0	0	0	0	0	96
1-BUTENE	kg/hr	0	0	0	0	0	0	0	0	0	1808	2997	2997	0	1212	0	0	1808	0	0	2997
BUTDIENE	kg/hr	0	0	0	0	0	0	0	0	0	21	34	34	0	14	0	0	21	0	0	34
CO2	kg/hr	0	0	3723	0	0	0	0	0	0	320	501	501	0	184	0	0	321	0	0	501
CO	kg/hr	0	0	0	0	0	0	0	0	0	68	106	106	0	39	0	0	68	39	38	106
O2	kg/hr	0	0	343	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N2	kg/hr	0	0	15364	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARGON	kg/hr	0	0	250	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CHAR	kg/hr	0	0	0	0	0	0	0	0	0	0	299	299	296	3	3	299	0	0	0	0

b. Process area: Phase Separation

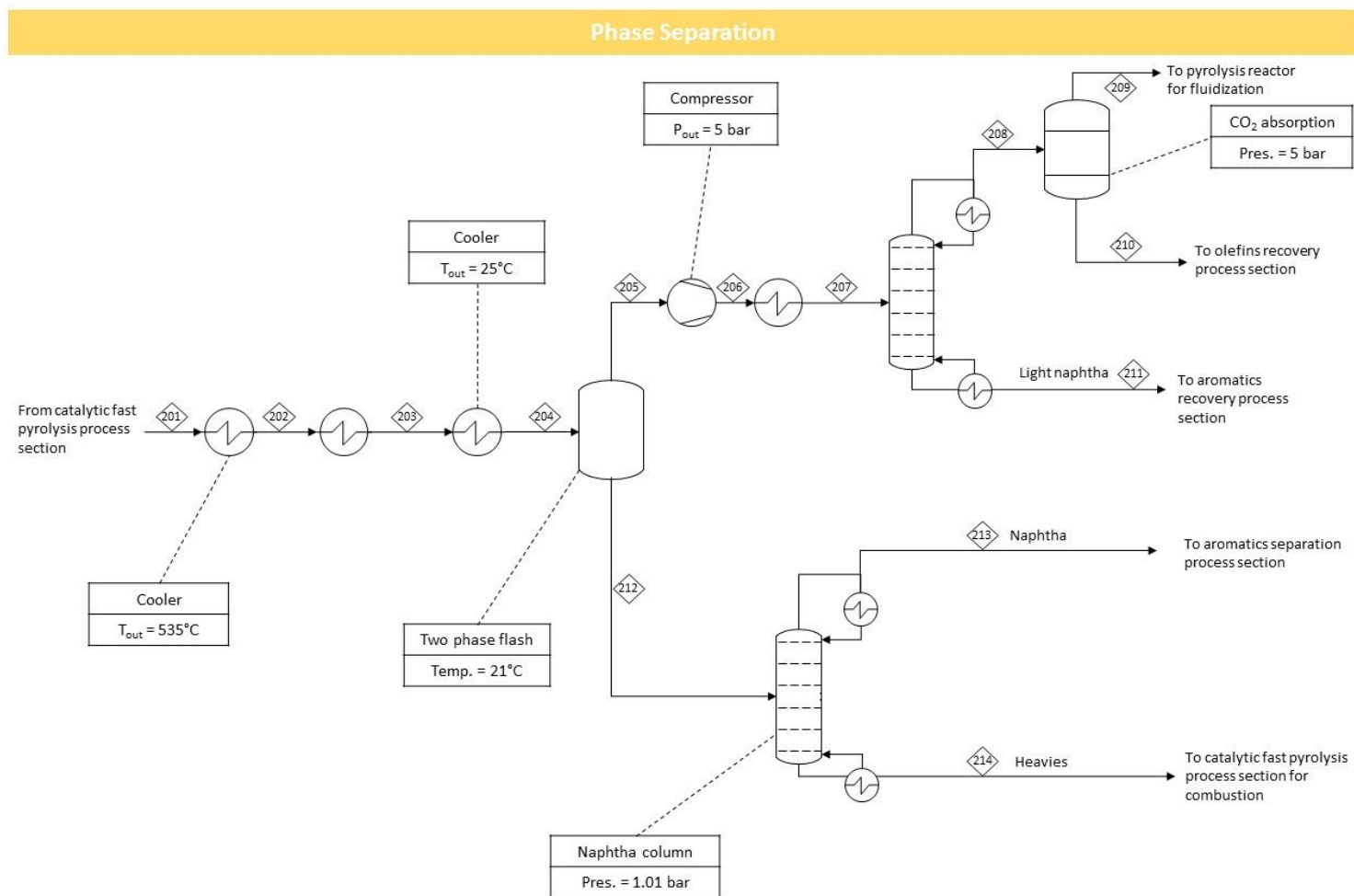


Fig. S2. Detailed PFD of pyrolysis phase separation into liquid and gaseous stream rich in aromatics and olefins, respectively (base case). Mixed plastic wastes and other raw inputs are shown in red; intermediate, recycle, and waste streams are shown in black.

Streams composition

Components	Units	201	202	203	204	205	206	207	208	209	210	211	212	213	214
Total Flow	kg/hr	17103	17103	17103	17103	12103	12103	12103	7800	4104	199	5000	4350	650	17103
Volume Flow	l/min	477036	438514	179325	132532	129965	25835	23527	16636	8352	5	107	91	19	477036
Temperature	°C	670	594	90	25	25	43	23	22	22	21	21	20	275	670
Pressure	bar	1	1	1	1	1	5	5	5	5	5	1	1	1	1
H2	kg/hr	38	38	38	38	14	14	14	14	14	0	0	0	0	38
CH4	kg/hr	405	405	405	405	146	146	146	146	146	0	0	0	0	405
C2H6	kg/hr	248	248	248	248	89	89	89	89	89	0	1	1	0	248
C3H8	kg/hr	778	778	778	778	279	279	279	279	275	4	10	10	0	778
C2H4	kg/hr	1833	1833	1833	1833	659	659	659	659	658	1	3	3	0	1833
C3H6	kg/hr	4201	4201	4201	4201	1506	1506	1506	1506	1490	16	43	43	0	4201
HCl	kg/hr	946	946	946	946	332	332	332	332	316	16	51	51	0	946
C4H10	kg/hr	31	31	31	31	8	8	8	8	5	3	15	15	0	31
N-C6H14	kg/hr	121	121	121	121	17	17	17	17	7	10	91	91	0	121
C7H14	kg/hr	205	205	205	205	37	37	37	37	19	17	133	133	0	205
BENZENE	kg/hr	654	654	654	654	48	48	48	48	12	36	584	584	0	654
TOLUENE	kg/hr	1368	1368	1368	1368	33	33	33	33	3	29	1330	1330	0	1368
XYLENE	kg/hr	1050	1050	1050	1050	13	13	13	13	1	12	1036	1036	0	1050
CUMENE	kg/hr	240	240	240	240	10	10	10	10	2	8	227	227	0	240
N-C8H18	kg/hr	378	378	378	378	4	4	5	5	0	4	373	373	0	378
N-C9H20	kg/hr	126	126	126	126	0	0	0	0	0	0	125	125	0	126
N-C10H22	kg/hr	168	168	168	168	0	0	0.2	0.2	0	0	168	168	0	168
C11H24	kg/hr	10	10	10	10	0	0	0	0	0	0	10	10	0	10
C12H26	kg/hr	1	1	1	1	0	0	0	0	0	0	1	1	0	1
C13H28	kg/hr	570	570	570	570	0	0	0	0	0	0	569	15	554	570
C15H32	kg/hr	96	96	96	96	0	0	0	0	0	0	96	0	96	96
C24H50	kg/hr	2997	2997	2997	2997	1058	1058	1058	1058	1016	42	132	131	0	2997
1-BUTENE	kg/hr	34	34	34	34	12	12	12	12	12	1	2	2	0	34
BUTDIENE	kg/hr	501	501	501	501	180	180	180	0	0	0	1	1	0	501
CO2	kg/hr	106	106	106	106	38	38	38	38	38	0	0	0	0	106
CO	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARGON	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CHAR	kg/hr	17103	17103	17103	17103	12103	12103	12103	7800	4104	199	5000	4350	650	17103

c. Process area: Olefins Recovery

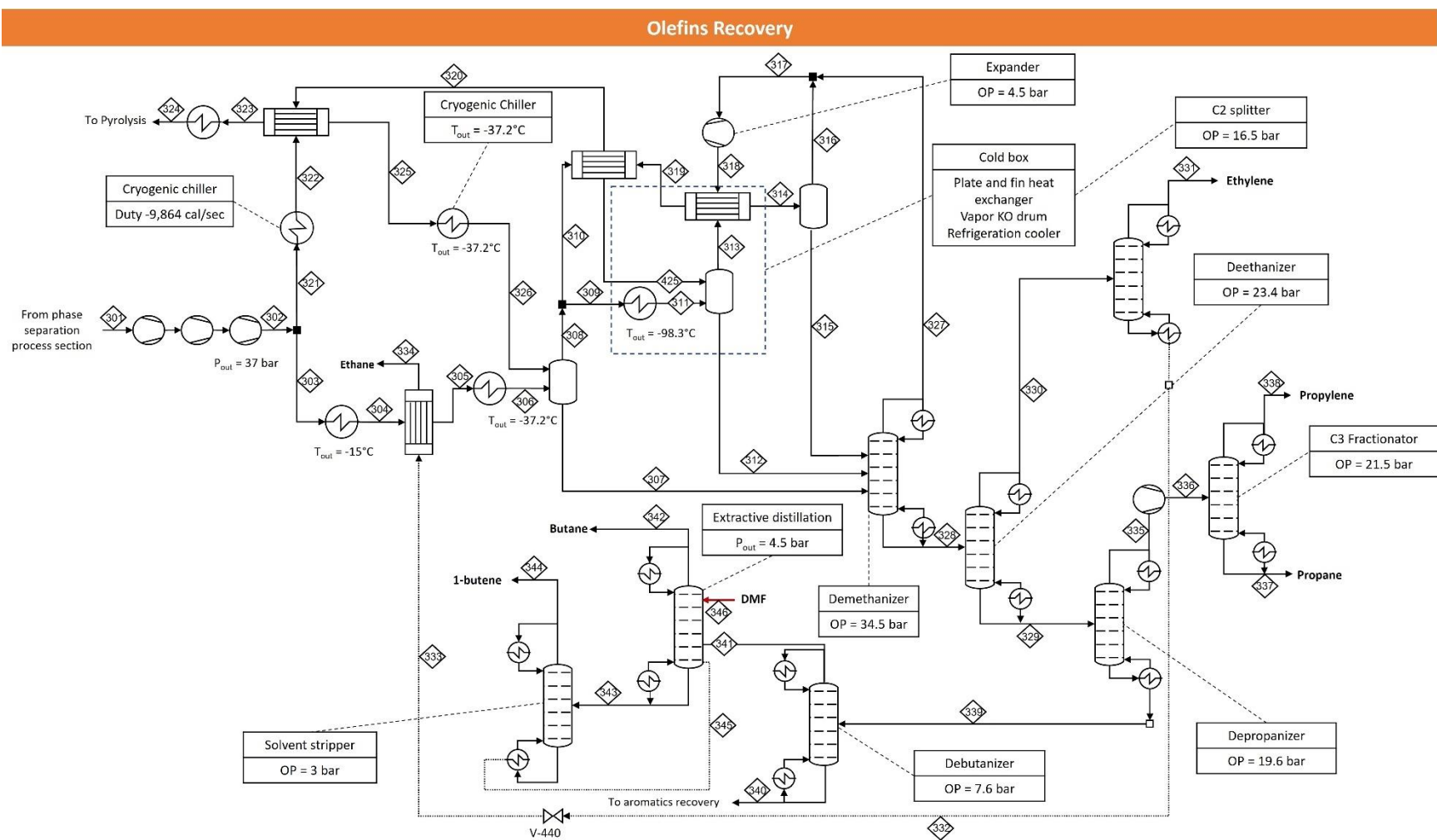


Fig. S3. Detailed PFD of recovery of olefins from the gaseous stream of the pyrolysis effluent (base case). Mixed plastic wastes and other raw inputs are shown in red; intermediate, recycle, and waste streams are shown in black.

Streams composition

Components	Units	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323
Mass Flows	kg/hr	4104	4104	3612	3612	3612	3612	4005	100	78	22	78	44	56	56	14	42	222	222	222	222	493	493	222
Volume Flow	l/min	8352	576	506	195	190	166	118	70	55	15	34	1	42	31	1	31	105	649	721	765	69	23	789
Temperature	°C	22	50	50	-15	-18	-37	-37	-37	-37	-98	-98	-98	-129	-129	-129	-97	-141	-133	-128	50	-31	-126	
Pressure	bar	5	38	38	38	38	37	37	37	37	37	37	37	37	37	37	34	4	4	4	4	38	38	4
H2	kg/hr	14	14	12	12	12	12	5	9	7	2	7	0	9	9	0	9	14	14	14	14	2	2	14
CH4	kg/hr	146	146	128	128	128	128	114	31	24	7	24	6	25	25	6	19	146	146	146	146	17	17	146
C2H6	kg/hr	89	89	78	78	78	78	87	2	2	1	2	2	0	0	0	0	0	0	0	0	11	11	0
C3H8	kg/hr	275	275	242	242	242	242	274	1	1	1	1	0	0	0	0	0	0	0	0	0	33	33	0
C2H4	kg/hr	658	658	579	579	579	579	629	29	22	6	22	22	7	7	6	1	25	25	25	25	79	79	25
C3H6	kg/hr	1490	1490	1312	1312	1312	1312	1481	10	7	2	7	9	0	0	0	0	0	0	0	0	179	179	0
C4H10	kg/hr	316	316	278	278	278	278	316	0	0	0	0	0	0	0	0	0	0	0	0	0	38	38	0
N-C6H14	kg/hr	5	5	4	4	4	4	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0
C6H12	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C7H14	kg/hr	7	7	6	6	6	6	7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0
BENZENE	kg/hr	19	19	17	17	17	17	19	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	0
TOLUENE	kg/hr	12	12	11	11	11	11	12	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0
XYLENE	kg/hr	3	3	3	3	3	3	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N-C8H18	kg/hr	2	2	1	1	1	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N-C10H22	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N-C9H20	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CUMENE	kg/hr	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C11H24	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C12H26	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C13H28	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C15H32	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C20H42	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C24H50	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1-BUTENE	kg/hr	1016	1016	894	894	894	894	1015	1	1	0	1	1	0	0	0	0	0	0	0	0	122	122	0
BUTDIENE	kg/hr	12	12	10	10	10	10	12	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0
CO2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	kg/hr	38	38	34	34	34	34	22	16	12	3	12	1	15	15	1	14	38	38	38	38	5	5	38
O2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
DMF	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Components	Units	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346
Mass Flows	kg/hr	222	493	493	180	3882	3170	712	636	76	76	76	1781	1781	277	1504	1388	56	1333	315	8080	1022	7058	4
Volume Flow	l/min	1594	23	23	69	147	116	260	343	3	18	86	678	632	11	518	50	1	42	534	173	2691	155	125
Temperature	°C	12	-34	-37	-87	58	75	-20	-35	-14	-37	-36	49	54	61	52	108	141	61	47	120	47	197	25
Pressure	bar	4	37	37	34	34	23	23	17	17	8	8	20	21	21	21	20	8	8	5	5	3	3	1
H2	kg/hr	14	2	2	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CH4	kg/hr	146	17	17	127	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2H6	kg/hr	0	11	11	0	89	11	78	4	74	74	74	11	11	0	11	0	0	0	0	0	0	0	0
C3H8	kg/hr	0	33	33	0	275	275	0	0	0	0	0	275	275	266	9	0	0	0	0	0	0	0	0
C2H4	kg/hr	25	79	79	24	633	1	632	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0
C3H6	kg/hr	0	179	179	0	1490	1488	2	0	2	2	2	1488	1488	5	1484	0	0	0	0	0	0	0	0
C4H10	kg/hr	0	38	38	0	316	316	0	0	0	0	0	0	0	0	0	316	3	313	313	0	0	0	0
N-C6H14	kg/hr	0	1	1	0	5	5	0	0	0	0	0	0	0	0	0	5	5	0	0	0	0	0	0
C6H12	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C7H14	kg/hr	0	1	1	0	7	7	0	0	0	0	0	0	0	0	7	7	0	0	0	0	0	0	0
BENZENE	kg/hr	0	2	2	0	19	19	0	0	0	0	0	0	0	0	0	19	19	0	0	0	0	0	0
TOLUENE	kg/hr	0	1	1	0	12	12	0	0	0	0	0	0	0	0	0	12	12	0	0	0	0	0	0
XYLENE	kg/hr	0	0	0	0	3	3	0	0	0	0	0	0	0	0	0	3	3	0	0	0	0	0	0
N-C8H18	kg/hr	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0	0	0
N-C10H22	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N-C9H20	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CUMENE	kg/hr	0	0	0	0	1	1	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
C11H24	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C12H26	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C13H28	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C15H32	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C20H42	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C24H50	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1-BUTENE	kg/hr	0	122	122	0	1016	1016	0	0	0	0	6	6	6	6	0	1010	3	1008	0	1008	1008	0	0
BUTDIENE	kg/hr	0	1	1	0	12	12	0	0	0	0	0	0	0	0	0	11	0	11	1	10	10	0	0
CO2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	kg/hr	38	5	5	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
DMF	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	7062	4	7058	4

d. Process area: Aromatic Hydrocarbons Recovery

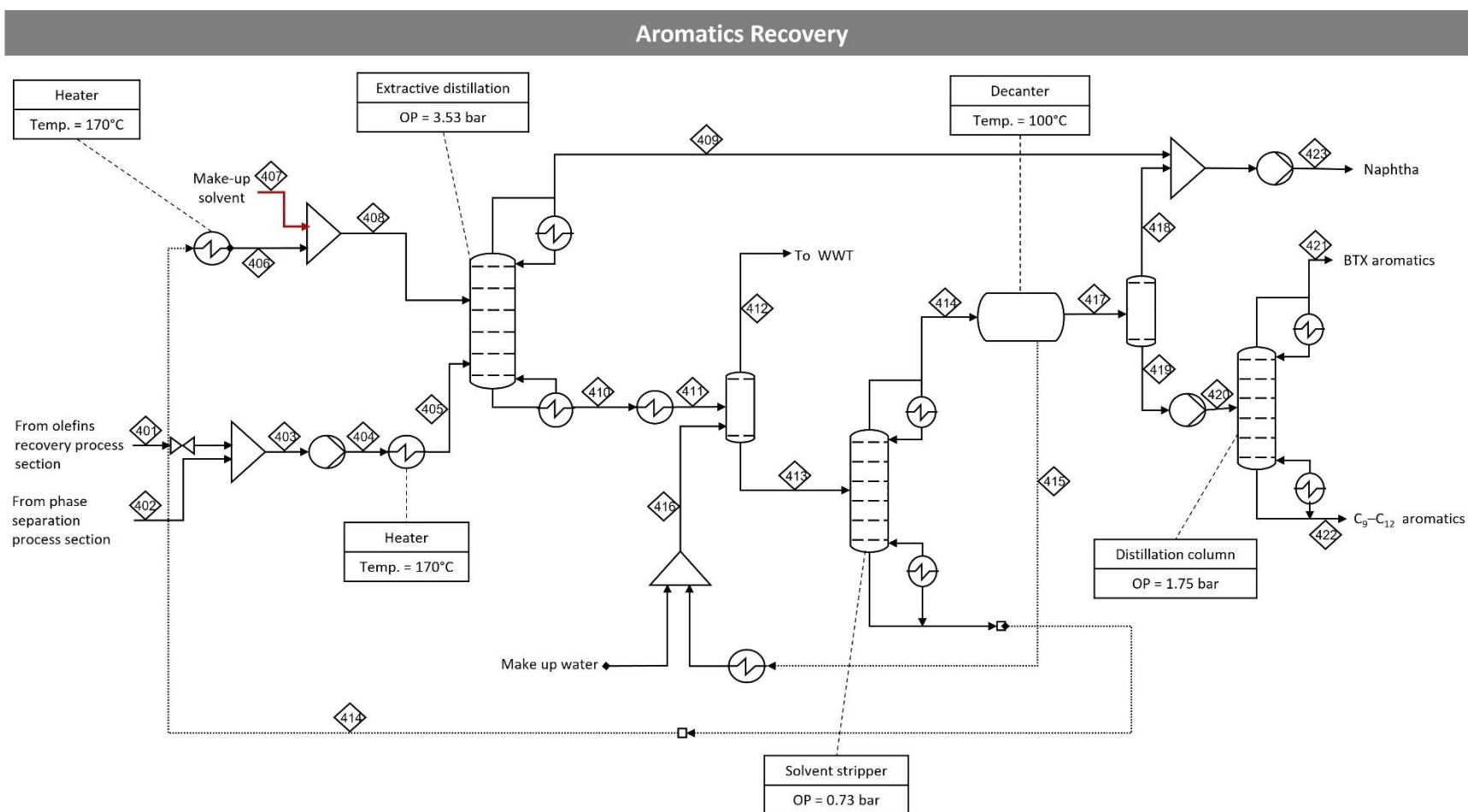


Fig. S4. Detailed PFD of the aromatic hydrocarbons recovery process section (base case). Mixed plastic wastes and other raw inputs are shown in red; intermediate, recycle, and waste streams are shown in black.

Streams composition

Components	Units	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423
Mass Flows	kg/hr	56	4350	4406	4406	4406	10086	21	10106	363	14149	14149	397	14126	10086	196	996	3845	859	2986	2986	1971	1015	1844
Volume Flow	l/min	1	91	95	92	2418	161	0	161	9	277	238	7	232	171	4	17	85	272	63	63	44	24	855
Temperature	°C	141	20	21	22	170	170	160	170	4	232	90	72	72	233	100	37	100	99	99	99	147	175	61
Pressure	bar	8	1	1	4	4	4	4	4	4	4	1	1	1	1	1	1	1	1	1	2	2	2	1
H2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CH4	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C2H6	kg/hr	0	1	1	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
C3H8	kg/hr	0	10	10	10	10	0	0	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	10
C2H4	kg/hr	0	3	3	3	3	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	3
C3H6	kg/hr	0	43	43	43	43	0	0	0	43	0	0	0	0	0	0	0	0	0	0	0	0	0	43
C4H10	kg/hr	3	51	54	54	54	0	0	0	54	0	0	0	0	0	0	0	0	0	0	0	0	0	54
N-C6H14	kg/hr	5	15	20	20	20	0	0	0	2	18	18	0	9	0	0	0	9	9	0	0	0	0	20
C6H12	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C7H14	kg/hr	7	91	98	98	98	0	0	0	98	98	0	98	0	1	1	97	97	0	0	0	0	0	98
C8H16	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C9H18	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C11H22	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BENZENE	kg/hr	19	133	153	153	153	0	0	0	111	42	42	0	42	0	0	0	42	0	42	42	42	0	111
TOLUENE	kg/hr	12	584	596	596	596	0	0	0	2	594	594	0	588	0	0	0	588	0	588	588	588	0	8
XYLENE	kg/hr	3	1330	1333	1333	1333	0	0	0	0	1333	1333	0	1320	0	0	0	1320	0	1320	1320	1317	3	13
N-C8H18	kg/hr	2	227	228	228	228	0	0	0	0	228	228	0	228	0	0	0	228	228	0	0	0	0	228
N-C10H22	kg/hr	0	125	125	125	125	1024	0	1024	0	1149	1149	0	1149	1024	0	0	125	125	0	0	0	0	125
N-C9H20	kg/hr	0	373	373	373	373	25	0	25	0	398	398	0	398	25	0	0	373	373	0	0	0	0	373
CUMENE	kg/hr	1	1036	1036	1036	1036	246	0	246	0	1283	1283	0	1283	246	0	0	1036	0	1036	1036	24	1013	0
C11H24	kg/hr	0	168	168	168	168	0	0	0	0	168	168	0	0	0	0	0	0	0	0	0	0	0	168
C12H26	kg/hr	0	10	10	10	10	0	0	0	0	10	10	0	0	0	0	0	0	0	0	0	0	0	10
C13H28	kg/hr	0	1	1	1	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1
C15H32	kg/hr	0	15	15	15	15	0	0	0	0	15	15	0	0	0	0	0	0	0	0	0	0	0	15
C20H42	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C24H50	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1-BUTENE	kg/hr	3	132	134	134	134	0	0	0	134	0	0	0	0	0	0	0	0	0	0	0	0	0	134
BUTDIENE	kg/hr	0	2	2	2	2	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2
CO2	kg/hr	0	1	1	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
CO	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O2	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SULFOLAN	kg/hr	0	0	0	0	0	8790	21	8811	0	8811	8811	0	8812	8790	2	2	20	20	0	0	0	0	21
DMF	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

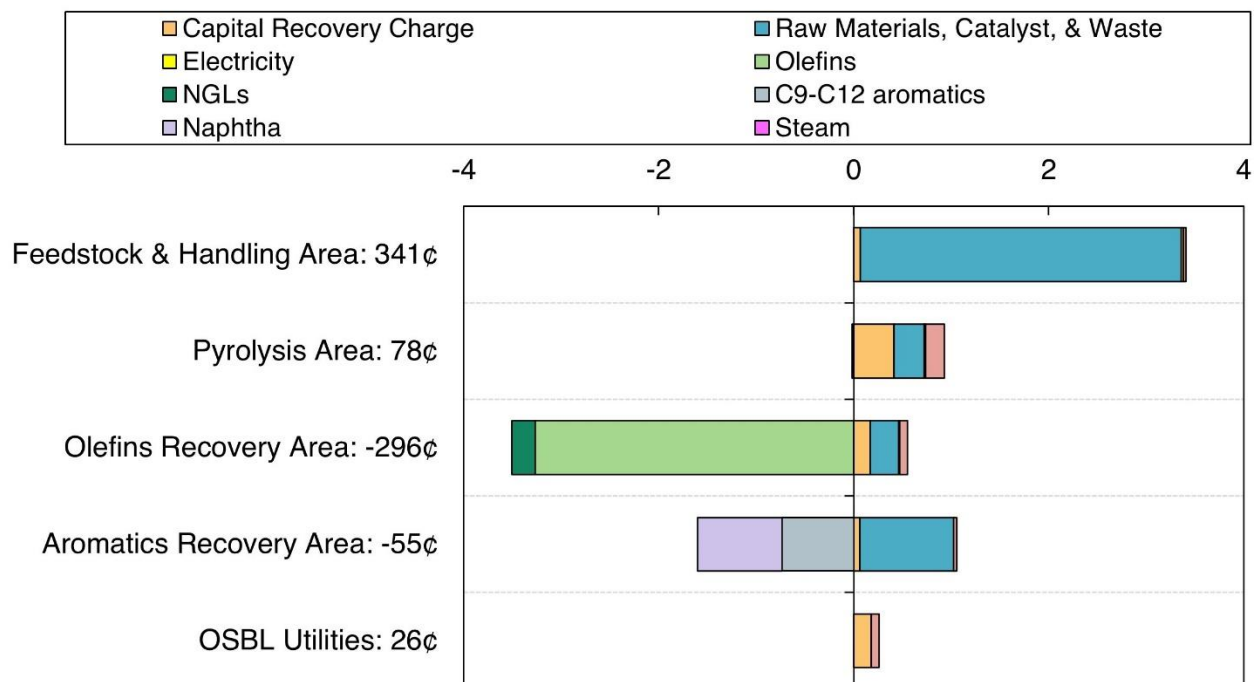


Fig. S5. Operating expense breakdown by process area (Case B – mixed product).

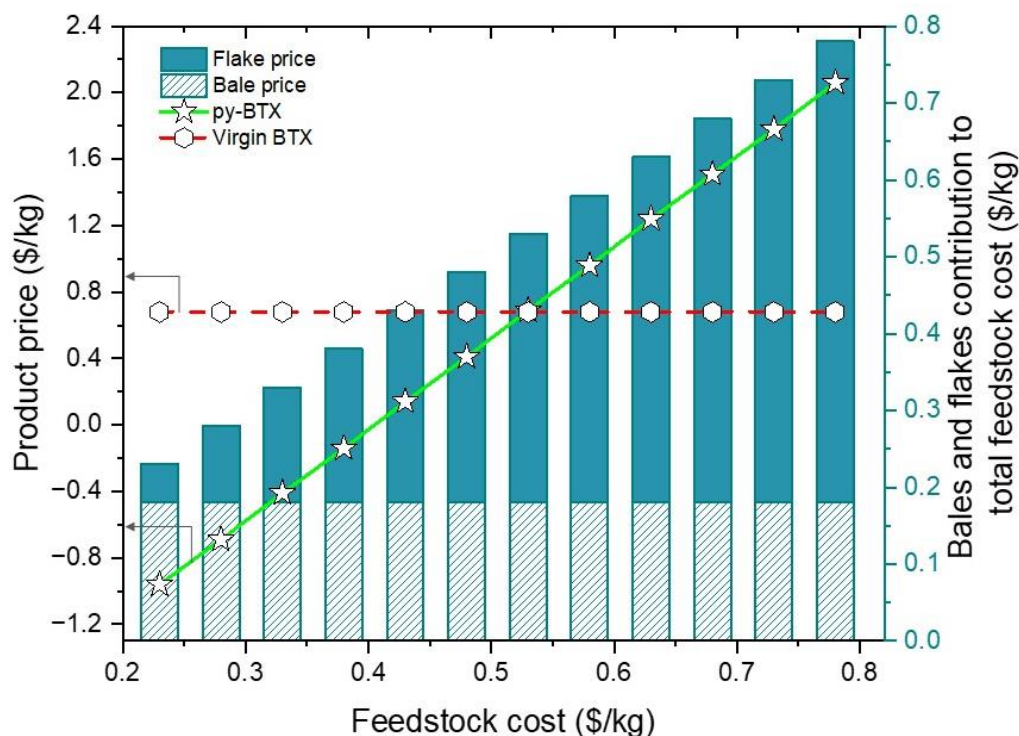


Fig. S6. MSP of BTX product as a function of feedstock cost, which is the total of the costs for plastic bales and flakes. Here, when the price of bales is fixed at \$0.18/kg, the effect of variations in the cost of flakes is seen on the overall MSP of BTX.

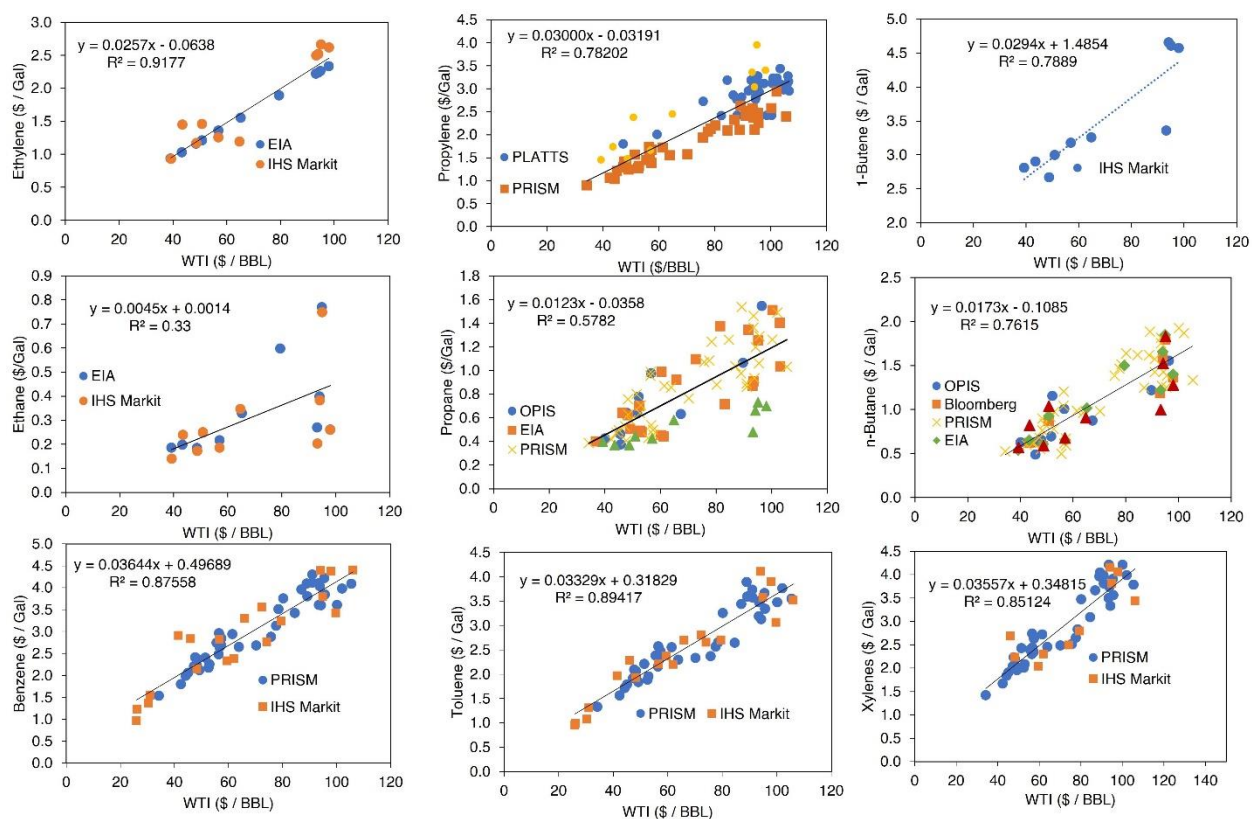


Fig. S7. Example of how product pricing values were determined based on historical WTI crude oil price. The data points used to develop the pricing equations represent snapshots derived from the open literature.¹ First, historical prices of WTI crude oil are plotted against the different petrochemical products. Then, linear regression is performed to obtain the slope and intercept values. These values are used to obtain the price of a particular petrochemical product at a designated WTI crude oil price as seen in **Fig. S8**.

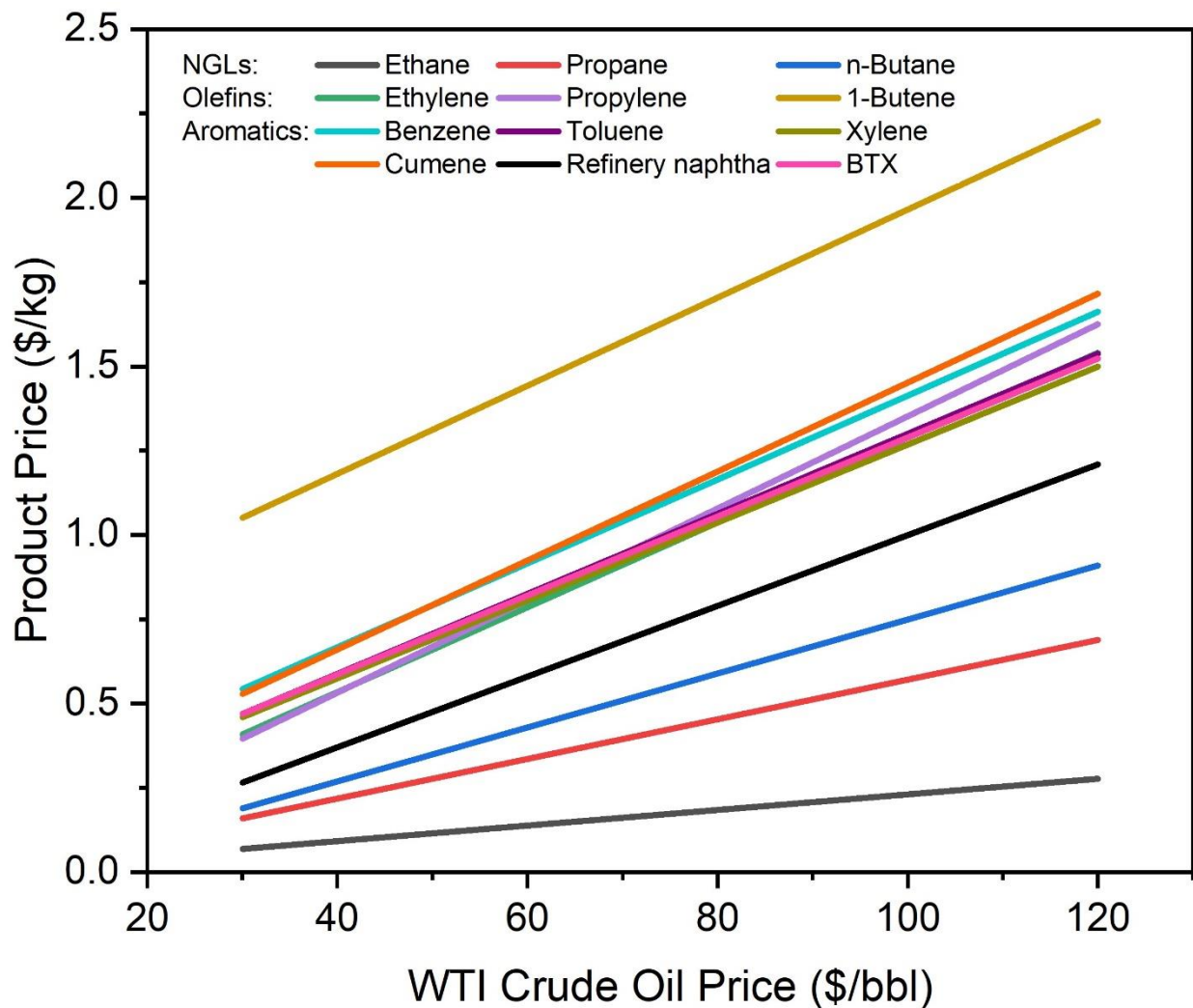


Fig. S8. Trends of price change of different products in this study vis-à-vis WTI crude oil price. The graph shows a comparison between trendlines for different products. These trendlines were obtained through the linear regression of historical price data for WTI crude oil and different petrochemical products from 2010 to 2020. WTI crude oil price varied from \$30/bbl to \$120/bbl.

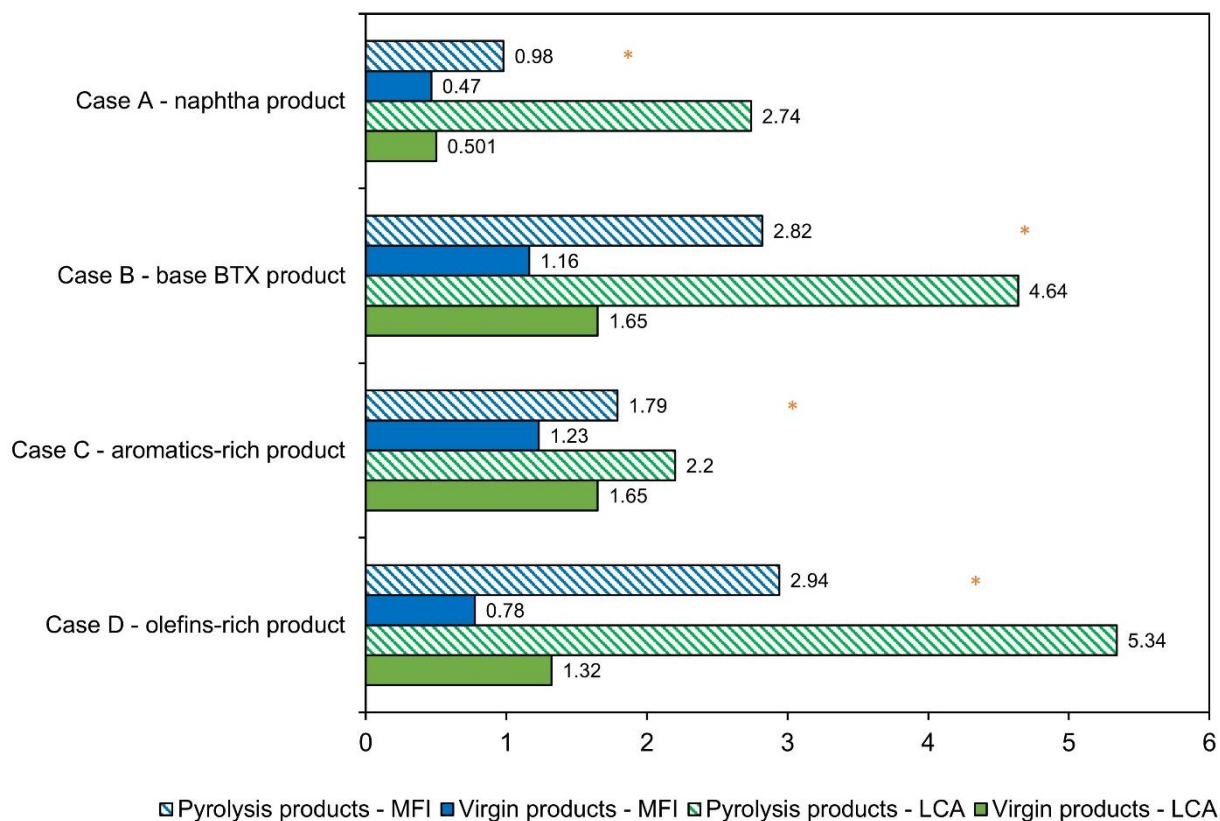


Fig. S9. Comparison of GHG emissions from the catalytic fast pyrolysis of mixed plastic wastes by MFI and LCA for Case A – naphtha product, Case B – mixed product, Case C – aromatics-rich product, and Case D – olefins-rich product. The differences between MFI and LCA results can be attributed to several factors. First, MFI does not consider process emissions arising from the pyrolysis reaction (0.88 kg CO₂/kg naphtha for Case A, 1.85 kg CO₂/kg BTX for Case B, 1.23 kg CO₂/kg BTX for Case C, and 1.40 kg CO₂/kg ethylene for Case D) or from virgin petrochemical manufacture (e.g., ~0.6-1.1 kg CO₂/kg ethylene), resulting in lower GHG estimates. The MFI results would increase significantly upon inclusion of these stoichiometric emissions, as shown by the asterisk marks on the graph. Second, MFI and LCA use different background datasets. MFI models United States specific production pathways based on the latest industrial information from IHS Markit, whereas the ecoinvent database in LCA is typically generalized globally. The same process component (e.g., steam or electricity) or co-product (e.g., propylene or propane) will therefore have different GHG emissions on a per kilogram basis when estimated with MFI or LCA. This is particularly evident in Case C, which generates large quantities of co-products with different environmental impacts; LCA provides negative credits of 3.89 kg CO₂ eq/kg and 0.501 kg CO₂ eq/kg for cumene and naphtha, respectively, in comparison to 2.49 kg CO₂ eq/kg and 0.455 kg CO₂ eq/kg in MFI.

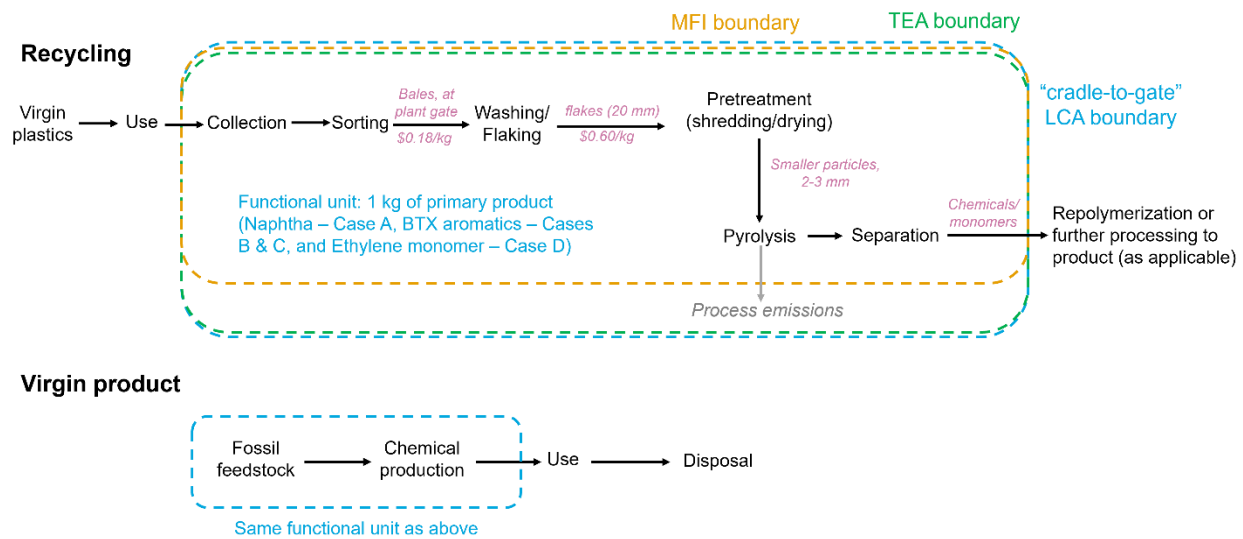


Fig. S10. MFI, LCA, and TEA system boundaries for the four catalytic fast pyrolysis-based mixed plastic waste recycling scenarios, as well as for the corresponding virgin materials (naphtha in Case A, BTX aromatic hydrocarbons in Cases B & C, and ethylene monomer in Case D).

B. Supporting tables

Feedstock composition: The typical composition of MPW stream globally consists of at least 70% polyolefins such as HDPE, LDPE, LLDPE, and PP.²⁻⁶ In addition to these four polymers, MPW also contains co-mingled plastic types (1–7 resin identification code) in the form of bottles, films, containers, etc. In household applications, PET is primarily used in bottles, containers, textiles, and carpeting, while HDPE is used in injection/blow-molded bottles, containers, toys, pipe systems, etc. Post-consumer plastic waste contains more HDPE than PET because of higher production volumes of HDPE, different collection systems for bottles/beverage containers, and different methodologies for classification of plastics products from EPA (e.g., carpets and rugs are classified separately from plastics products). Combined, recycled PET and HDPE account for nearly 99% of the total bottles recycled. The feedstock is modeled here as being procured from a local MRF at \$0.18/kg as bales and converted to flakes at an additional price of \$0.42/kg with the composition shown in **Table S1**.

Table S1. Feedstock composition.⁷

Component	Weight % (dry basis)
HDPE	19%
LDPE	21%
LLDPE	18%
PP	24%
PS	11%
PET	3%
PVC	4%
Moisture	<1%

Table S2. Financial parameters used in discounted cash flow rate of return (DCFROR) analysis.

Discounted Cash Flow Financial Parameters		
Equity	(% of FCI)	40%
Loan Interest		8.0%
Loan Term, years		10
Working Capital	(% of FCI)	5.00%
Discount Rate (IRR)		10%
Income Tax Rate		21%
Plant Depreciation Period	(Years)	7
Plant Life	(Years)	30
Construction Period	(Years)	3
% Spent in Year -2		8%
% Spent in Year -1		60%
% Spent in Year 0		32%
Start-up Time	(Years)	0.50
BTX production year 1	(% of Normal Capacity)	50%
Variable Costs	(% of Normal)	75%
Fixed Cost	(% of Normal)	100%
Land Requirement	Acres	10
Land Cost	\$/acre	\$14,000

Case A – Naphtha Product

Table S3. Economic summary for naphtha production (Case A – naphtha product).

PRODUCTION OF NAPHTHA FROM THE PYROLYSIS OF MIXED PLASTICS WASTE			
Feed Pretreatment, Catalytic Fast Pyrolysis, and Phase Separation			
All Values in 2016\$			
Minimum Naphtha Selling Price (MSP)		\$2.18	/kg
Contributions:	Feedstock	\$1.58	/kg
	Naphtha Conversion	\$0.60	/kg
	Naphtha Production	34.3	MMkg per year
	Naphtha Yield	\$0.40	Tonnes naphtha/tonne MPW feed
	Feedstock + Handling Cost	\$600	/MT feedstock
	Internal Rate of Return (After-Tax)	10%	
	Equity Percent of Total Investment	40%	
Capital Costs		Manufacturing Costs (cents/kg naphtha)	
A100: Feedstock Pretreatment	\$4,161,035	Feedstock + Handling	152
A200: Catalytic Fast Pyrolysis	\$26,057,722	Catalyst cost	6
A300: Pyrolysis Vapor Quench	\$2,137,285	OSBL Utilities	7.8
OSBL (25% of ISBL)	\$8,089,011	Electricity (import)	2
Total Installed Equipment Cost	\$40,445,053	Other Raw Materials	0
Additional Direct Costs (17.5% of ISBL)	\$5,662,307	Waste Disposal	0.8
Total Direct Costs (TDC)	\$46,107,360	Coproducts	0
Land and Working Capital	\$3,828,589	Fixed Costs	18.7
Indirect Costs (60% of TDC)	\$27,664,416	Capital Depreciation	7.3
Total Capital Investment (TCI)	\$77,600,365	Average Income Tax	2.1
		Average Return on Investment	21.6
		Total	218.31
		Manufacturing Costs (\$/yr)	
Installed Equipment Cost/Annual kg	\$1.18	Feedstock + Handling	\$52,100,000
Total Capital Investment/Annual kg	\$2.26	Catalyst Cost	\$2,000,000
		OSBL Utilities	\$2,700,000
		Electricity (import)	\$700,000
		Other Raw Materials	\$0
		Waste Disposal	\$300,000
		Coproducts	\$0
Operating Hours Per Year (On-Stream Factor)	7884 (90%)	Fixed Costs	\$6,400,000
Loan Rate	8%	Capital Depreciation	\$2,500,000
Term (years)	10	Average Income Tax	\$700,000
Capital Charge Factor (Computed)	0.14	Average Return on Investment	\$7,400,000
		Total	\$74,800,000

Case B – mixed product (base case with BTX aromatic hydrocarbons as principal product)

Total capital investment

Table S4. Capital investment breakdown by process sections for the Case B – mixed product (base case). All costs are in USD.

Equipment ID	Equipment Type	Installation Factor	Capital Cost (2016\$)	
			Equipment Cost*	Installed Cost*
Feedstock Pretreatment				
CB-104	Heated screw conveyor	1.82	107,000	195,000
FH-110	Feed hopper/storage	1.41	1,085,000	1,528,000
CB-101	Feed conveyor	1.85	109,000	201,000
R-101	PVC dechlorination reactor	4.01	270,000	1,171,000
MT-130	HCl mixing tank	5.50	17,000	107,000
M-120	Shredder	1.70	140,000	238,000
M-104A	Cross flow pellet dryer	2.00	14,000	27,000
	Balance of plant		348,000	694,000
	Feedstock pretreatment total (\$)		2,091,000	4,161,000
Catalytic Fast Pyrolysis				
R-201	Fluidized bed reactor	4.00	3,492,000	13,970,000
R-202	Char combustor	3.97	51,000	202,000
K-202	Combustor air compressor	1.60	284,000	454,000
K-201	Fluidizing gas recycle compressor	1.60	422,000	675,000
R-202C	Catalyst cooler	3.00	588,000	1,764,000
T-201	Catalyst steam stripper	3.00	411,000	1,232,000
R-203	Fired heater	1.31	1,314,000	4,005,000
	Balance of plant		2,291,930	8,005,561
	Catalytic Fast Pyrolysis Total (\$)		7,881,573	24,030,630
Phase Separation				
E-301	Reactor effluent cooler	2.03	76,000	154,000
E-302	Reactor effluent cooler	2.00	149,000	250,527
E-303	Reactor effluent cooler	2.00	40,000	81,000
T-304	2-phase flash vessel (V/L)	4.99	225,000	1,122,000

D-305	Naphtha column	2.13	104,000	221,000
	Balance of Plant		119,000	375,000
	Phase separation total (\$)		713,000	2,251,000
	Olefins separation			
K-401	Compressor	2.15	1,469,000	2,351,000
E-401	Cooler	3.23	16,000	52,000
D-401	Naphtha column	2.77	63,000	175,000
E-402	Recycle cooler	3.23	1,000	4,000
T-401	Demethanizer	1.91	259,000	517,000
T-401C	T-410C – Demethanizer-condenser	4.58	1,000	4,000
T-401B	T-410B – Demethanizer-reboiler	2.83	13,000	36,000
T-402	Deethanizer column	1.60	240,000	410,000
T-401C	T-402C – Condenser (startup)	4.58	3,000	15,000
T-402B	T-402C – Reboiler (startup)	2.83	11,000	30,000
D-403	C2 splitter	1.91	256,000	424,000
D-403C	D-403C – Condenser (startup)	6.66	7,000	46,000
D-403B	D-403B – Reboiler (startup)	2.83	15,000	41,000
T-404	Depropanizer	2.15	162,000	303,000
T-404C	T-404C – Condenser (startup)	4.58	8,000	37,000
T-404B	T-404C – Reboiler (startup)	2.83	25,000	70,000
D-405	C3 fractionator	1.91	1,113,000	1,446,000
D-405C	D-405C – Condenser (startup)	6.66	29,000	192,000
D-405B	D-405C – Reboiler (startup)	2.83	62,000	174,000
T-406	Debutanizer	1.91	75,000	197,000
T-406	T-406C – Condenser (startup)	4.58	5,000	24,000
T-406	T-406C – Reboiler (startup)	2.83	13,000	35,000
K-402	Compressor	2.15	109,000	234,000
C2REC	Heat exchanger	3.17	69,000	218,000
Chiller-5	Refrigeration cooler	3.23	12,000	40,000
Chiller-1	Refrigeration cooler	3.23	45,000	145,000
Chiller-2	Refrigeration cooler	3.23	15,000	47,000

Chiller-3	Refrigeration cooler	3.23	4,000	12,000
Chiller-4	Refrigeration cooler	3.23	1,000	3,000
V-401	Vapor KO drum	3.45	1,000	4,000
V-402	Vapor KO drum	3.45	1,000	3,000
V-403	Vapor KO drum	3.45	1,000	2,500
CB1	BAHX- Heat exchanger	4.58	77,000	243,000
CB2	BAHX- Heat exchanger	4.58	69,000	218,000
CB3	BAHX- Heat exchanger	4.58	64,000	204,000
E-403	Cooler	3.23	8,000	26,000
T-407	Extractive distillation column	1.19	405,000	482,000
T-407C	T-407 Condenser (startup)	4.58	46	210
T-407B	T-407 Reboiler (startup)	2.83	16,000	45,000
D-408	Stripper	1.69	126,000	171,000
D-408C	D-408 Condenser (startup)	4.58	3,000	13,000
D-408B	D-408 Reboiler (startup)	2.83	4,000	10,000
	Balance of plant	0.35	1,462,000	1,473,000
	Olefins separation total (\$)		6,333,000	10,179,000
	Aromatics Extraction			
D-501	Extractive distillation column	1.69	338,000	571,000
D-501C	D-501 Condenser (startup)	4.58	3,000	15,000
D-501B	D-501 Reboiler (startup)	2.83	17,000	50,000
T-502	Wash column	2.00	4,000	8,000
D-503	Solvent stripper	2.27	104,000	237,000
D-503C	D-503 Condenser (startup)	6.66	21,000	142,000
D-503B	D-503 Reboiler (startup)	2.83	56,000	158,000
D-504	Decanter	1.82	3,000	6,000
E-501	Cooler	3.23	49,000	159,000
E-502	Heater	3.23	72,000	232,000
E-503	Cooler	3.23	111,000	359,000
E-504	Cooler	3.23	2,000	5,000
T-504	Cumene column	1.42	564,000	801,000

T-504C	T-504C condenser	6.66	12,000	82,000
T-504B	T-504B Reboiler	2.83	29,000	81,000
	Balance of plant	0.3	416,000	872,000
	Aromatics recovery total (\$)		1,802,000	3,777,000
	OSBL			
	Outside battery limits capital (25% of ISBL)		4,800,000	11,200,000
	OSBL total (\$)		4,800,000	11,200,000
	TOTAL (\$)		23,900,000	55,900,000
	Total Direct Costs (TDC)			63,700,000
	Total Indirect Costs			38,300,000
	Fixed Capital Investment (FCI)			101,800,000
	Total Capital Investment (TCI)			107,000,000

*These values are rounded off to the nearest integer.

Table S5. CAPEX breakdown for the base case, related to **Fig. 4a** from main text.

Process Section	\$M	% TIC
Feedstock Pretreatment	4.2	7%
Catalytic Fast Pyrolysis	24.0	43%
Pyrolysis Vapor Quench	2.3	4%
Olefins Separation	10.4	19%
Aromatics Separation	3.8	7%
OSBL	11.2	20%
Total Installed Cost	55.8	100%

Table S6. Cost factors for indirect costs.

Indirect Costs	% of TDC
Prorated expenses	10.0
Field expenses	10.0
Home office and construction fee	20.0
Project contingency	10.0
Other costs (start-ups, Permits, etc.)	10.0
Total Indirect Costs	60.0

*Excluding land purchase cost

Table S7. Annual operating cost by process section for the base case, related to **Fig. 4b** in the main text.

Process Area	Yearly Operating Expenses Breakdown (\$M/year)							
	Feedstock	Catalyst	Operational Costs	Solvent	Electricity	Co-products	Fixed Costs	Total
Feedstock Pre-processing	52.14	0.00	0.40	0.00	0.32	0.00	0.00	52.86
Catalytic Fast Pyrolysis	0.00	2.05	0.05	0.00	0.27	-0.27	0.00	2.10
Phase Separation	0.00	0.00	1.04	0.00	0.00	0.00	0.00	1.04
Olefins Separation	0.00	0.00	4.05	0.01	0.21	-55.55	0.00	-51.29
Aromatics Separation	0.00	0.00	4.04	10.94	0.00	-25.40	0.00	-10.43
Fixed Costs	0.00	0.00	0.00	0.00	0.00	0.00	8.76	8.76
Total	52.14	2.05	9.58	10.94	0.81	-81.22	8.76	3.05

Table S8. Basis of product and co-product's application, annual global consumption (in million metric tons), and pricing.⁸⁻¹¹

Products and co-products	Application/use	Global consumption (MM metric tons)	Price (\$/kg)	Pricing Justifications
BTX aromatic hydrocarbons	plastics	150	0.68	As blends of fuels to boost octane number or as petrochemical material
Naphtha	fuel	341	0.38	To replace crude oil-based naphtha
Ethylene	plastics	174.5	0.58	For making plastics (HDPE, LDPE)
Propylene	plastics	120.8	0.83	For making plastics (HDPE, LDPE)
Butene	plastics	53.8	1.27	For making plastics (HDPE, LDPE)
Ethane	refrigerant	100	0.17	As a working fluid in the refrigeration cycle of air conditioning systems and heat pumps
Propane	fuel	68	0.33	Used as fuel for cooking, engine applications
Butane	fuel	26	0.36	Fuel for portable stoves, heating fuel, refrigerant
Other aromatics (mainly cumene)	plastics	16.4	0.64	Chemical intermediate in the production of phenol and acetone, which are in turn used to make plastics

Table S9. Economic summary for BTX aromatics production in the base case (Case B – mixed product).

PRODUCTION OF BTX AROMATICS FROM THE CATALYTIC PYROLYSIS OF MIXED PLASTICS WASTE			
Feed Pretreatment, Catalytic Fast Pyrolysis and Phase Separation, Olefins Recovery, and Aromatics Extraction			
All Values in 2016\$			
Minimum BTX Selling Price (MSP)		\$1.07	/kg
Contributions:	Feedstock	\$3.42	/kg
	BTX Conversion	\$2.76	/kg
	Olefins Co-product Conversion	\$-3.27	/kg
	Naphtha Co-product Conversion	\$-0.87	/kg
	NGLs Co-product Conversion	\$-0.24	/kg
	Other Aromatics Co-product Conversion	\$-0.73	/kg
	BTX Production	15.83	MMkg per year
	BTX Yield	0.20	tonnes BTX/tonne MPW
	Olefins Co-product Production	25.26	MMkg per year
	Olefins Co-product Yield	0.32	tonnes / tonne MPW feed
	Naphtha Co-product Production	16.35	MMkg per year
	Naphtha Co-product Yield	0.21	tonnes / tonne MPW feed
	NGLs Co-product Production	5.32	MMkg per year
	NGLs Co-product Yield	0.07	tonnes /tonne MPW feed
	Other Aromatics Co-product Production	8.15	MMkg per year
	Other Aromatics Co-product Yield	0.10	tonnes /tonne MPW feed
	Feedstock + Handling Cost	\$600	/ MT feedstock
	Internal Rate of Return (After-Tax)	10%	
	Equity Percent of Total Investment	40%	
Capital Costs		Manufacturing Costs (cents/kg BTX)	
A100: Feedstock Pretreatment	\$4,161,035	Feedstock + Handling	329.4
A200: Catalytic Fast Pyrolysis	\$24,030,630	Catalyst cost	12.9
A300: Pyrolysis Vapor Quench	\$2,250,946	OSBL Utilities	54.1
A400: Olefins Separation	\$10,424,021	Electricity (import)	5.1
A500: Aromatics Separation	\$3,777,442	Other Raw Materials	73.0
OSBL (25% of ISBL)	\$11,161,018	Waste Disposal	2.5
Total Installed Equipment Cost	\$55,805,092	Coproducts	-513.1
Additional Direct Costs (17.5% of ISBL)	\$7,812,713	Fixed Costs	55.3
Total Direct Costs (TDC)	\$63,617,805	Capital Depreciation	21.5
Land and Working Capital	\$5,229,424	Average Income Tax	6.5
Indirect Costs (60% of TDC)	\$38,170,683	Average Return on Investment	59.8
Total Capital Investment (TCI)	\$107,017,912	Total	107.1
		Manufacturing Costs (\$/yr)	
Installed Equipment Cost/Annual kg	\$3.53	Feedstock + Handling	\$52,100,000
Total Capital Investment/Annual kg	\$6.76	Catalyst Cost	\$2,000,000
		OSBL Utilities	\$8,600,000
		Electricity (import)	\$800,000
		Other Raw Materials	\$11,600,000
Operating Hours Per Year (On-Stream Factor)	7,884 (90%)	Waste Disposal	\$400,000
Loan Rate	8%	Coproducts	\$81,200,000
Term (years)	10	Fixed Costs	\$8,800,000
Capital Charge Factor (Computed)	0.13	Capital Depreciation	\$3,400,000
		Average Income Tax	\$1,000,000
		Average Return on Investment	\$9,500,000
		Total	\$17,000,000

Table S10. Salary cost for plant employees.

Position	Salary (2016)	Number of Positions	Total Cost (2016)
Plant Manager	147,000	1	147,000
Plant Engineer	70,000	1	70,000
Maintenance Supervisor	57,000	1	57,000
Maintenance Technician	40,000	6	240,000
Lab Manager	56,000	1	56,000
Laboratory Technician	40,000	1	40,000
Shift Supervisor	48,000	3	144,000
Shift Operators	40,000	12	480,000
Yard Employees	28,000	4	112,000
Clerks & Secretaries	36,000	1	36,000
Total Salaries (2016\$/yr)			1,382,000
Labor Burden	90% of Total Salaries		1,243,800
			2,625,000

Note: Labor costs are indexed, if necessary, to values from the U.S. Bureau of Labor Statistics (<http://data.bls.gov/cgi-bin/srgate> CEU3232500008).

Table S11. Fixed operating costs.

Cost Item	Factor	Total Cost (2016) \$
Labor Burden	90% of Total Salaries	1,244,000
Overhead and Benefits	90% of Labor and Supervision	2,363,000
Maintenance	3.0% of fixed capital investment (FCI*)	3,054,000
Property Insurance and Tax	0.7% of fixed capital investment (FCI*)	713,000
Total Fixed Operating Costs		7,374,000

*Percentage of FCI exclude land purchase cost

Table S12. Operating costs and summary of variable operating cost additions.

Component	Cost (2016\$)	Source
Mixed Plastic Waste	\$0.60/kg	RecyclingMarkets.net ⁸
Sulfolane	\$63.8/kg	Industry database ⁹
Dimethyl formamide	\$0.81/kg	PEP Year Handbook ¹⁰
Steam	HP: \$17.6/1000 kg, MP: \$15.3/1000 kg LP: \$13.2/1000 kg	Seider <i>et al.</i> 2017 Textbook ¹¹
Natural Gas	\$0.26/kg (\$5/MMBtu)	Dutta <i>et al.</i> 2015 Design Report ¹²
Process Water	\$0.27/m ³	Seider <i>et al.</i> 2017 Textbook ¹¹
Cooling Water	Inlet: 25 °C; Outlet: 30 °C	Calculated based on volumetric flow (m ³ /s) as described in Ulrich and Vasudevan ¹³
62.5% Spent FCC Catalyst	\$2.98/kg (includes catalyst recovery cost)	CatCost Estimate ¹⁴
37.5% ZSM-5 Zeolite Catalyst	\$2.98/kg (includes catalyst recovery cost)	CatCost Estimate ¹⁴
Refrigerants	Temperature: -102°C, -40.03°C, -18°C, -7°C	Calculated based on cooling capacity (kJ/s) of refrigerant as described in Ulrich and Vasudevan ¹³
Electricity	\$0.068/kWh	Seider <i>et al.</i> ¹¹

Table S13. Simplified breakdown of the MSP of BTX in the base case (Case B – mixed product), related to **Fig. 4c** in the main text.

Cost Category	Cost Contribution (\$/kg _{BTX})
Feedstock Cost	3.29
Catalyst cost	0.13
OSBL Utilities	0.54
Electricity Cost	0.05
Other raw materials	0.73
Other Operating Cost	0.63
Fixed Cost	0.55
Capital Charge	0.27
Co-product Credits	-5.13
MSP	1.07

Table S14. Minimum selling price of BTX by process section for the base case (Case B – mixed product), related to **Fig. 4c**.

Process Area	Cost Category (\$/kg BTX)							
	Feedstock	Catalyst	Operational Costs	Capital Charge	Solvent	Electricity	Co-products	Total
Feedstock Pre-processing	3.29	0.00	0.04	0.07	0.00	0.02	0.00	3.42
Catalytic Fast Pyrolysis	0.00	0.13	0.27	0.38	0.00	0.02	-0.02	0.77
Pyrolysis Vapor Quench	0.00	0.00	0.09	0.04	0.00	0.00	0.00	0.12
Olefins Separation	0.00	0.00	0.36	0.164	0.00	0.01	-3.51	-2.97
Aromatics Separation	0.00	0.00	0.29	0.06	0.69	0.00	-1.60	-0.56
OSBL	0.00	0.00	0.11	0.18	0.00	0.00	0.00	0.29
Total	3.29	0.13	1.16	0.88	0.69	0.05	-5.13	1.07

Selection of sensitivity analysis parameters

Table S15. Rationale for choosing the low and high values for the univariate sensitivity analysis, related to **Fig. 5a** in the main text.

Sensitivity Analysis Parameter (Best case*: Base Case: Worst Case)	Justification for the high and low values of parameters
Feedstock Cost (\$/kg) 0.5: 0.6: 0.7	<p>Best case: Lower cost sources of polyolefins such as films and flexibles that are currently discarded.</p> <p>Base case: Based on RecyclingMarkets.net estimates for the price of mixed plastics waste (bales) and its conversion to flakes. Feedstock contains at least 80% polyolefins.</p> <p>Worst case: Poor sorting (at MRF) and collection (from municipalities) scenario for the typical feedstock composition of the base case.</p>
Downstream Capital (%) 0: base: +100	<p>Best case: No capital investment for products separation due to integration in existing petroleum refineries.</p> <p>Base case: greenfield plant</p> <p>Worst case: Uncertainty in capital expenditure</p>
Internal Rate of Return (%) 5: 10: 15	<p>Best case: Low risk investment assuming the technology is mature with well-established markets for the different products and co-products.</p> <p>Base case: The standard discount rate for medium risk projects.</p> <p>Worst case: High risk projects with new products yet to find a niche in market.</p>
Operating Cost (M\$) (-22%, base, +22%)	<p>Best case: Energy integration leads to lower utilities usage causing a drop in operating expenses.</p> <p>Base case: Standard separation approaches for olefins and aromatics.</p> <p>Worst case: Reflects potential underestimation of auxiliary utilities to the plant.</p>
Sulfolane cost (\$/kg) 43.8: 63.8: 81.4	<p>Best case: 99.9% purity (0.07% water). Extractive distillation solvent, polymerization solvent.</p> <p>Base case: 97.1% purity (2.9% water). Extraction of aromatic hydrocarbons from oil refinery stream.</p> <p>Worst case: 97.1% purity (2.9% water) for use as plasticizer and curing agent.</p>
CFP reactor cost (%) -20, base, +40	<p>Best case: Mature technology.</p> <p>Base case: Based on product mass flows designed for fluidized bed reactor technology.</p> <p>Worst case: Uncertainty in capital cost estimation of the pyrolysis reactor, as capital cost is often underestimated for emerging technologies.</p>
Catalyst loading (%) 1: 6: 12	<p>Best case: For aromatics yield improvement (tradeoff with olefins)</p> <p>Base case: For olefins and aromatics production.</p> <p>Worst case: For olefins yield improvement (tradeoff with aromatics).</p>
Plant size (tpd) 500: 240: 100	<p>Best case: Modular design enable the installation of multiple units and benefits from economies-of-scale.</p> <p>Base case: Size of a typical commercial scale pyrolysis plant in operation to-date (e.g., Ensyn, Brightmark).</p> <p>Worst case: Typical size of demonstration plants.</p>
Catalyst cost (\$/kg) 2.43: 2.98: 6.75	<p>Best case: Step method – uses costs in \$/hr for synthesis steps run at a contract manufacturer.</p> <p>Base case: CapEx & OpEx Factors method – uses process design literature for a dedicated, new build catalyst plant.</p> <p>Worst case: ZSM-5 with rare earth metals.</p>
Time on stream (%) 94: 90: 86	<p>Best case: 343 days of plant operation (22 days for maintenance).</p> <p>Base case: 328.5 days of plant operation (36.5 days for maintenance).</p> <p>Worst case: 314 days of plant operation (51 days for maintenance).</p>

Income Tax Rate (%) 15: 21: 35	Best case: Aggressive tax rate. Base case: Nominal tax rate. Worst case: Conservative tax rate.
Working Capital (% FCI) 5: 5: 10	Best case: Nominal WC for the operation of one month of plant. Base case: Nominal WC for the operation of one month of plant. Worst case: Uncertain future calamities might render i

*Best case refers to parameters that result in lower MSP values

Table S16. Sensitivity results for change to MSP BTX aromatic hydrocarbons, related to **Fig. 5a**.

Sensitivity Analysis Parameter (low cost: base case: high cost)	Change to MSP – BTX aromatic hydrocarbons (\$/kg)	
	Low cost	High cost
Feedstock Cost (\$/kg) 0.5: 0.6: 0.7	-\$0.55	\$0.55
Downstream Capital (%) 0: base: +100	\$0.73	\$1.42
Internal Rate of Return (%) 5: 10: 15	-\$0.28	\$0.29
Operating Expense (% M\$) -5: base: +5	-\$0.15	\$0.31
Sulfolane Cost (\$/kg) 43.8: 63.8: 81.4	-\$0.22	\$0.19
CFP Reactor Cost (%) -20, base, +40	-\$0.08	\$0.16
Catalyst Loading (%) 1: 6: 12	-\$0.11	\$0.13
Plant Size (tpd) 500: 240: 100	-\$0.15	\$0.06
Catalyst Cost (\$/kg) 2.43: 2.98: 6.75	-\$0.02	\$0.17
Time on Stream (%) 94: 90: 86	-\$0.07	\$0.08
Income Tax Rate (%) 15: 21: 35	-\$0.02	\$0.06
Working Capital (% FCI) 5: 5: 10	\$0.00	\$0.04

Case C – Aromatics rich product

Table S17. Economic summary for BTX aromatic hydrocarbons production (Case C – aromatics rich product).

PRODUCTION OF BTX AROMATICS (BTX) FROM THE PYROLYSIS OF MIXED PLASTICS WASTE (MPW)			
Feed Pretreatment, Catalytic Pyrolysis, Vapor Quench, Olefins Recovery, and Aromatics Extraction			
All Values in 2016\$			
Minimum BTX Selling Price (MSP)		\$0.95	/kg
Contributions:	Feedstock	\$2.29	/kg
	BTX Conversion	\$1.75	/kg
	Olefins Co-product Conversion	\$-1.52	/kg
	Naphtha Co-product Conversion	\$-0.71	/kg
	NGLs Co-product Conversion	\$-0.12	/kg
	Other Aromatics Co-product Conversion	\$-0.73	/kg
	BTX Production	23.58	MMkg per year
	BTX Yield	0.30	Tonnes BTX/tonne feed
	Olefins Co-product Production	15.88	MMkg per year
	Olefins Co-product Yield	0.20	tonnes / tonne MPW feed
	Naphtha Co-product Production	20.11	MMkg per year
	Naphtha Co-product Yield	0.26	tonnes / tonne MPW feed
	NGLs Co-product Production	3.87	MMkg per year
	NGLs Co-product Yield	0.05	Tonnes /tonne MPW feed
	Other Aromatics Co-product Production	12.15	MMkg per year
	Other Aromatics Co-product Yield	0.15	tonnes/tonne MPW feed
	Feedstock + Handling Cost	\$600	/MT feedstock
	Internal Rate of Return (After-Tax)	10%	
	Equity Percent of Total Investment	40%	
Capital Costs		Manufacturing Costs (cents/kg BTX)	
A100: Feedstock Pretreatment	\$4,161,035	Feedstock + Handling	221.1
A200: Catalytic Fast Pyrolysis	\$24,735,394	Catalyst cost	8.7
A300: Pyrolysis Vapor Quench	\$1,688,686	OSBL Utilities	46.2
A400: Olefins Separation	\$8,834,774	Electricity (import)	2.9
A500: Aromatics Separation	\$4,581,411	Other Raw Materials	32.6
OSBL (25% of ISBL)	\$11,000,325	Waste Disposal	7.9
Total Installed Equipment Cost	\$55,001,624	Coproducts	-309.4
Additional Direct Costs (17.5% of ISBL)	\$7,700,227	Fixed Costs	26.9
Total Direct Costs (TDC)	\$62,701,851	Capital Depreciation	14.0
Land and Working Capital	\$5,156,148	Average Income Tax	4.3
Indirect Costs (60% of TDC)	\$37,621,111	Average Return on Investment	39.6
Total Capital Investment (TCI)	\$105,479,110	Total	94.7
		Manufacturing Costs (\$/yr)	
Installed Equipment Cost/Annual kg	2.33	Feedstock + Handling	\$52,100,000
Total Capital Investment/Annual kg	4.47	Catalyst Cost	\$2,000,000
		OSBL Utilities	\$10,900,000
		Electricity (import)	\$700,000
		Other Raw Materials	\$7,700,000
Operating Hours Per Year (On-Stream Factor)	7,884 (90%)	Waste Disposal	\$1,900,000
Loan Rate	8%	Coproducts	\$-73,000,000
Term (years)	10	Fixed Costs	\$6,300,000
Capital Charge Factor (Computed)	0.13	Capital Depreciation	\$3,300,000
		Average Income Tax	\$1,000,000
		Average Return on Investment	\$9,300,000
		Total	\$22,200,000

Case D – Olefins rich product

Table S18. Economic summary for ethylene production (Case D – olefins rich product).

PRODUCTION OF ETHYLENE FROM THE PYROLYSIS OF MIXED PLASTICS WASTE (MPW) Feed Pretreatment, Catalytic Pyrolysis, Vapor Quench, Olefins recovery, and Aromatics Extraction All Values in 2016\$			
Minimum Ethylene Selling Price (MSP)		\$0.85	/kg
Contributions:	Feedstock	\$5.54	/kg
	Ethylene Conversion	\$4.37	/kg
	Olefins Co-product Conversion	\$-6.88	/kg
	Naphtha Co-product Conversion	\$-1.22	/kg
	NGLs Co-product Conversion	\$-0.87	/kg
	Other Aromatics Co-product Conversion	\$-0.09	/kg
	Ethylene Production	9.7	MMkg per year
	Ethylene Yield	0.12	Tonnes Ethylene/tonne feed
	Olefins Co-product Production	31.6	MMkg per year
	Olefins Co-product Yield	0.40	tonnes / tonne MPW feed
	Naphtha Coproduct Production	15.1	MMkg per year
	Naphtha Co-product Yield	0.19	tonnes / tonne MPW feed
	NGLs Co-product Production	11.48	MMkg per year
	NGLs Co-product Yield	0.15	Tonnes /tonne MPW feed
	Other Aromatics Co-product Production	0.38	MMkg per year
	Other Aromatics Co-product Yield	0.005	tonnes/tonne MPW feed
	Feedstock + Handling Cost	\$600	/MT feedstock
	Internal Rate of Return (After-Tax)	10%	
	Equity Percent of Total Investment	40%	
Capital Costs		Manufacturing Costs (cents/kg Ethylene)	
A100: Feedstock Pretreatment	\$4,161,035	Feedstock + Handling	535.3
A200: Catalytic Fast Pyrolysis	\$26,883,043	Catalyst cost	101.5
A300: Pyrolysis Vapor Quench	\$2,592,147	OSBL Utilities	104.9
A400: Olefins Separation	\$12,793,216	Electricity (import)	9.4
A500: Aromatics Separation	\$2,369,374	Other Raw Materials	11.6
OSBL (25% of ISBL)	\$12,199,704	Waste Disposal	5.3
Total Installed Equipment Cost	\$60,998,518	Coproducts	-907.2
Additional Direct Costs (17.5% of ISBL)	\$8,539,792	Fixed Costs	69.2
Total Direct Costs (TDC)	\$69,538,310	Capital Depreciation	38.0
Land and Working Capital	\$5,703,065	Average Income Tax	11.5
Indirect Costs (60% of TDC)	\$41,722,986	Average Return on Investment	105.3
Total Capital Investment (TCI)	\$116,964,361	Total	84.9
		Manufacturing Costs (\$/yr)	
Installed Equipment Cost/Annual kg	6.26	Feedstock + Handling	\$52,100,000
Total Capital Investment/Annual kg	12.01	Catalyst Cost	\$9,900,000
		OSBL Utilities	\$10,200,000
		Electricity (import)	\$900,000
		Other Raw Materials	\$1,100,000
		Waste Disposal	\$500,000
		Coproducts	\$-88,400,000
		Fixed Costs	\$6,700,000
		Capital Depreciation	\$3,700,000
		Average Income Tax	\$1,100,000
		Average Return on Investment	\$10,300,000
		Total	\$8,100,000
Operating Hours Per Year (On-Stream Factor)	7,884 (90%)		
Loan Rate	8%		
Term (years)	10		
Capital Charge Factor (Computed)	0.13		

Table S19. MFI results on supply chain energy and GHG emissions for Case A – naphtha product, related to **Fig. 6b-c** in the main text.

	Supply Chain Energy Requirements (MJ/kg _{Naphtha})					
Case	Process Fuel	Fuel for Electricity	Renewable Electricity	Fuel for Transportation	Fuel as Chemical Feedstocks	Total Energy
Virgin naphtha	5.23	0.94	0.07	0.97	43.89	51.10
Case A – naphtha	11.1	7.31	0.37	2.65	6.50	28.0
	Supply Chain GHG Emissions (kg CO ₂ -eq/kg _{Naphtha})					
Case	Process Fuel	Electricity Generation	Transportation	Pyrolysis reaction emissions	Total GHG	
Virgin naphtha	0.31	0.07	0.09	data not available	0.47	
Case A – naphtha	0.74	0.52	0.22	0.88 (not included in the total at right)	0.98	

Table S20. MFI results on supply chain energy and GHG emissions for Case B – mixed product (base case), related to **Fig. 6b-c** in the main text. Here, the principal product is BTX mixture.

	Supply Chain Energy Requirements (MJ/kg _{BTX})					
Case	Process Fuel	Fuel for Electricity	Renewable Electricity	Fuel for Transportation	Fuel as Chemical Feedstocks	Total Energy
Virgin BTX aromatics	11	4.673	0.342	2.749	39.46	58.22
Case B – mixed product	22.2	12.5	0.572	5.31	3.73	44.4
	Supply Chain GHG Emissions (kg CO ₂ -eq/kg _{BTX})					
Case	Process Fuel	Electricity Generation	Transportation	Pyrolysis reaction emissions	Total GHG	
Virgin BTX aromatics	0.58	0.34	0.24	data not available	1.16	
Case B – mixed product	1.49	0.89	0.44	1.85 (not included in the total at right)	2.82	

Table S21. MFI results on supply chain energy and GHG emissions for Case C – aromatics-rich product, related to **Fig. 6b-c** in the main text.

	Supply Chain Energy Requirements (MJ/kg _{BTX})					
Case	Process Fuel	Fuel for Electricity	Renewable Electricity	Fuel for Transportation	Fuel as Chemical Feedstocks	Total Energy
Virgin BTX aromatics	10.92	5.38	0.39	3.09	35.68	55.46
Case C – BTX aromatics	19.2	7.96	0.345	3.53	2.47	28.1
	Supply Chain GHG Emissions (kg CO _{2-eq} /kg _{BTX})					
Case	Process Fuel	Electricity Generation	Transportation	Pyrolysis reaction emissions	Total GHG	
Virgin BTX aromatics	0.57	0.39	0.27	data not available	1.23	
Case C – BTX aromatics	0.93	0.56	0.30	1.23 (not included in the total at right)	1.79	

Table S22. MFI Results on supply chain energy and GHG emissions for Case D – olefins-rich product, related to **Fig. 6b-c** in the main text.

	Supply Chain Energy Requirements (MJ/kg _{Ethylene})					
Case	Process Fuel	Fuel for Electricity	Renewable Electricity	Fuel for Transportation	Fuel as Chemical Feedstocks	Total Energy
Virgin ethylene	8.72	2.16	0.16	1.49	46.03	58.56
Case D – ethylene	22.4	13.1	0.55	6.12	4.24	46.3
	Supply Chain GHG Emissions (kg CO _{2-eq} /kg _{Ethylene})					
	Process Fuel	Electricity Generation	Transportation	Pyrolysis reaction emissions	Total GHG	
Virgin ethylene	0.49	0.16	0.13	data not available	0.78	
Case D – ethylene	1.50	0.91	0.52	1.40 (not included in the total at right)	2.94	

Table S23. Life cycle assessment results for Case A – naphtha product in which pyrolysis of mixed plastic waste is used to produce naphtha, related to **Fig. 7a-b** in the main text. The results for fossil-based naphtha are included for comparison.

	<i>Impact category</i>										
	Acidification kg SO ₂ eq/kg	Carcinogenics CTUh/kg	Eco-toxicity CTUe/kg	Eutrophication kg N eq/kg	Fossil fuel depletion MJ surplus/kg	Global warming kg CO ₂ eq./kg	Non carcinogenic CTUh/kg	Ozone depletion kg CFC-11/kg	Particulates kg PM2.5 eq/kg	Smog kg O ₃ eq/kg	Water use m ³ /kg
<i>Case A: mixed plastic waste pyrolysis for naphtha</i>											
TOTAL	0.007	9.2E-8	51.6	0.0151	3.21	2.74	9.02E-7	3.53E-7	0.00248	0.0963	7.09
<i>Standard deviation</i>	<i>0.0008</i>	<i>6.15E-8</i>	<i>21.7</i>	<i>0.0062</i>	<i>0.401</i>	<i>0.073</i>	<i>4.46E-7</i>	<i>1.33E-7</i>	<i>0.00026</i>	<i>0.0076</i>	<i>9.4</i>
Process Emissions	0	0	0	0	0	0.877	0	0	0	0	0
Catalyst	2.39E-5	1.77E-10	0.023	1.51E-05	0.004	0.004	8.7E-10	5.41E-10	6.11E-06	0.0002	0.003
Cooling Water	5.34E-6	2.76E-10	0.020	4.53E-06	0.001	0.001	5.8E-10	1.09E-10	1.63E-06	7.69E-5	6.72
Process Water	4.05E-6	1.11E-10	0.006	2.98E-06	0.001	0.001	2.5E-10	2.85E-10	1.56E-06	4.63E-5	0.020
Methane	0.0006	2.08E-09	0.210	0.0002	0.690	0.049	7.93E-09	7.51E-08	8.03E-05	0.0037	0.020
Infrastructure	1.30E-7	4.36E-12	0.001	1.82E-07	1.11E-05	1.48E-05	3.9E-11	1.06E-12	3.09E-08	9.97E-7	4.0E-6
Steam	0.0007	2.50E-09	0.235	0.0002	0.323	0.172	1.04E-08	2.14E-08	6.97E-05	0.0051	0.009
Electricity	0.0007	1.53E-08	1.75	0.0016	0.149	0.196	5.23E-08	2.08E-08	0.0006	0.0050	0.033
Plastic feedstock	0.0050	7.15E-8	49.3	0.0131	2.04	1.44	8.29E-7	2.35E-7	0.00171	0.0822	0.295
Solids Disposal	8.23E-7	2.82E-11	2.13E-03	5.22E-06	8.42E-05	9.57E-05	5.0E-10	7.06E-12	1.57E-07	3.36E-5	1.7E-4
Wastewater	8.23E-7	2.82E-11	0.002	5.22E-06	8.42E-05	9.57E-05	5.0E-10	7.06E-12	1.57E-07	8.09E-6	-0.007
<i>Fossil-based naphtha</i>											
TOTAL	0.0053	1.77E-8	1.60	0.0019	8.04	0.501	6.60E-8	9.10E-7	0.0006	0.044	0.259
<i>Standard deviation</i>	<i>0.0018</i>	<i>2.12E-8</i>	<i>0.547</i>	<i>0.0005</i>	<i>0.198</i>	<i>0.0809</i>	<i>5.08E-8</i>	<i>4.95E-8</i>	<i>0.00015</i>	<i>0.0175</i>	<i>0.80</i>

Table S24. Life cycle assessment results for Case B – mixed product (base case) in which pyrolysis of mixed plastic waste is used to produce a benzene, toluene, and xylene mixture (BTX), related to **Fig. 7c-d** in the main text. The results for fossil-based BTX mixture are included for comparison.

	<i>Impact category</i>										
	Acidification kg SO ₂ eq/kg	Carcinogenics CTUh/kg	Eco-toxicity CTUe/kg	Eutrophication kg N eq/kg	Fossil fuel depletion MJ surplus/kg	Global warming kg CO ₂ eq./kg	Non carcinogenic CTUh/kg	Ozone depletion kg CFC- 11/kg	Particulates kg PM2.5 eq/kg	Smog kg O ₃ eq/kg	Water use m ³ /kg
<i>Case B: mixed plastic waste pyrolysis for BTX aromatics</i>											
TOTAL	0.0071	2.33E-7	119	0.042	-21.0	4.64	2.20E-6	-1.96E-7	0.00891	0.081	38.5
<i>Standard deviation</i>	<i>0.0032</i>	<i>2.53E-7</i>	<i>44.4</i>	<i>0.0187</i>	<i>2.4</i>	<i>0.412</i>	<i>1.09E-6</i>	<i>2.17E-7</i>	<i>0.00139</i>	<i>0.0274</i>	<i>52.0</i>
Process Emissions	0	0	0	0	0	1.85	0	0	0	0	0
Catalyst	5.17E-5	3.83E-10	0.051	3.27E-5	0.010	0.009	1.89E-9	1.17E-9	1.32E-5	0.0005	0.006
Cooling Water	3.12E-5	1.61E-9	0.117	2.65E-5	0.007	0.007	3.38E-9	6.36E-10	9.50E-6	0.0004	39.2
Process Water	2.22E-5	6.11E-10	0.034	1.64E-5	0.003	0.004	1.39E-9	1.57E-9	8.58E-6	0.0003	0.112
DMF	9.03E-6	6.23E-11	0.010	1.08E-5	0.005	0.001	4.0E-10	3.44E-10	1.62E-6	7.04E-5	0.001
Sulfolane	0.0003	7.80E-10	0.090	5.57E-5	0.073	0.015	3.54E-9	2.70E-9	4.04E-5	0.0007	0.026
Infrastructure	2.83E-7	9.43E-12	0.002	3.94E-7	2.40E-5	3.20E-5	8.4E-11	2.29E-12	6.69E-8	2.16E-6	8.6E-6
Steam	0.0067	2.52E-8	2.36	0.0016	3.25	1.73	1.05E-7	2.15E-7	0.0007	0.0508	0.091
Plastic feedstock	0.011	1.55E-7	107	0.0284	4.42	3.13	1.80E-6	5.08E-7	0.0037	0.178	0.639
Electricity	0.0018	3.82E-8	4.37	0.0040	0.372	0.488	1.31E-7	5.19E-8	0.0015	0.0125	0.081
Refrigeration	0.0066	1.40E-7	16.02	0.0145	1.36	1.79	4.79E-7	1.90E-7	0.0056	0.0458	0.297
Solids Disposal	5.56E-6	5.73E-10	2.80	0.0002	0.001	0.013	3.75E-8	1.16E-10	8.74E-7	7.28E-5	0.000
Wastewater	3.39E-6	1.16E-10	0.009	2.15E-5	0.000	0.000	2.06E-9	2.91E-11	6.48E-7	3.33E-5	-0.027
Aromatics (co-product)	-0.0050	-5.95E-8	-5.92	-0.0040	-4.85	-1.28	-1.96E-7	-5.91E-8	-0.0013	-0.0594	-0.775
Naphtha (co-product)	-0.0054	-1.82E-8	-1.65	-0.0019	-8.30	-0.518	-6.81E-8	-9.40E-7	-0.0006	-0.0455	-0.268
Ethylene (co-product)	-0.0063	-1.14E-8	-1.52	-0.0005	-3.70	-0.427	-5.20E-8	-3.88E-7	-0.0005	-0.0158	-0.064
Propylene (co-product)	-0.0030	-1.92E-8	-1.06	-0.0002	-7.35	-1.10	-9.36E-9	-3.94E-10	-0.0002	-0.0412	-0.366
Butene (co-product)	-0.0021	-1.51E-8	-0.867	-0.0001	-4.75	-0.789	-9.38E-9	-2.31E-9	-0.0002	-0.0284	-0.329
Ethane (co-product)	-0.0003	-1.35E-9	-0.123	-6.49E-5	-0.230	-0.029	-4.58E-9	-1.04E-8	-4.10E-5	-0.0016	-0.003
Propane (co-product)	-0.0008	-2.65E-9	-0.248	-0.0002	-1.01	-0.107	-1.11E-8	-1.13E-7	-9.35E-5	-0.0075	-0.031
Butane (co-product)	-0.0013	-5.52E-9	-0.506	-0.0003	-0.941	-0.120	-1.88E-8	-4.23E-8	-0.0002	-0.0065	-0.014
<i>Fossil-based BTX aromatics</i>											
TOTAL	0.0048	4.45E-8	2.18	0.0006	9.13	1.65	3.33E-8	1.42E-8	0.0004	0.066	1.28
<i>Standard deviation</i>	<i>9.50E-5</i>	<i>2.32E-8</i>	<i>2.52</i>	<i>0.00019</i>	<i>0.039</i>	<i>0.013</i>	<i>8.15E-8</i>	<i>7.16E-9</i>	<i>3.11E-5</i>	<i>0.0018</i>	<i>3.45</i>

Table S25. Life cycle assessment results for Case C – aromatics-rich product in which pyrolysis of mixed plastic waste is used to produce a benzene, toluene, and xylene mixture (BTX) under a high selectivity towards aromatics scenario, related to **Fig. 7e-f** in the main text. The results for fossil-based BTX aromatic hydrocarbons are included for comparison.

	<i>Impact category</i>										
	Acidif-ication kg SO ₂ eq/kg	Carcin-ogenics CTUh/kg	Eco-toxicity CTUe/kg	Eutro-plication kg N eq/kg	Fossil fuel depletion MJ surplus/kg	Global warming kg CO ₂ eq./kg	Non carcin-ogenic CTUh/kg	Ozone depletion kg CFC-11/kg	Particulates kg PM2.5 eq/kg	Smog kg O₃ eq/kg	Water use m ³ /kg
<i>Case C: mixed plastic waste pyrolysis for BTX aromatics (high aromatic selectivity)</i>											
TOTAL	-0.0006	8.26E-8	71.5	0.0205	-14.6	2.2	1.2E-6	-4.0E-7	0.00324	0.0589	14.2
<i>Standard deviation</i>	<i>0.00214</i>	<i>1.29E-7</i>	<i>30.0</i>	<i>0.0101</i>	<i>2.14</i>	<i>0.32</i>	<i>6.42E-7</i>	<i>3.45E-7</i>	<i>0.00077</i>	<i>0.0176</i>	<i>22.4</i>
Process Emissions	0	2.79E-12	0.000	0	0	1.27	7.9E-11	0	9.51E-7	0.0374	0
Catalyst	3.47E-5	2.57E-10	0.034	2.19E-5	0.006	0.006	1.27E-9	7.87E-10	8.89E-6	0.0003	0.004
Cooling Water	1.18E-5	6.11E-10	0.045	1.00E-5	0.003	0.003	1.28E-9	2.41E-10	3.60E-6	0.0002	14.9
Process Water	1.73E-5	4.76E-10	0.027	1.27E-5	0.003	0.003	1.08E-9	1.22E-9	6.68E-6	0.0002	0.087
DMF	2.37E-5	1.64E-10	0.027	2.83E-5	0.013	0.004	1.05E-9	9.03E-10	4.25E-6	0.0002	0.002
Sulfolane	0.0002	3.49E-10	0.040	2.49E-5	0.033	0.007	1.58E-9	1.21E-9	1.81E-5	0.0003	0.012
Infrastructure	1.90E-7	6.33E-12	0.001	2.65E-7	1.61E-5	2.15E-5	5.7E-11	1.54E-12	4.49E-8	1.45E-6	5.8E-6
Steam	0.0035	1.30E-8	1.22	0.0008	1.68	0.896	5.41E-8	1.11E-7	0.0004	0.0263	0.047
Plastic feedstock	0.0072	1.04E-7	71.7	0.0190	2.97	2.1	1.21E-6	3.41E-7	0.00248	0.120	0.429
Electricity	0.0010	2.17E-8	2.48	0.0022	0.211	0.277	7.41E-8	2.94E-8	0.0009	0.0071	0.046
Refrigeration	0.0021	4.48E-8	5.12	0.0046	0.435	0.572	1.53E-7	6.07E-8	0.0018	0.0146	0.095
Solids Disposal	3.73E-6	3.85E-10	1.88	0.0001	0.001	0.008	2.52E-8	7.77E-11	5.87E-7	4.89E-5	0.000
Wastewater	2.27E-6	7.76E-11	0.006	1.44E-5	0.000	0.000	1.38E-9	1.94E-11	4.33E-7	2.23E-5	-0.018
Aromatics (co-product)	-0.0050	-5.95E-8	-5.93	-0.0040	-4.85	-1.28	-1.97E-7	-5.92E-8	-0.0013	-0.0594	-0.775
Naphtha (co-product)	-0.0045	-1.51E-8	-1.36	-0.0016	-6.85	-0.428	-5.63E-8	-7.77E-7	-0.0005	-0.0375	-0.221
Ethylene (co-product)	-0.0019	-3.38E-9	-0.451	-0.0002	-1.10	-0.127	-1.54E-8	-1.15E-7	-0.0002	-0.0047	-0.019
Propylene (co-product)	-0.0009	-5.92E-9	-0.326	-5.42E-5	-2.27	-0.338	-2.89E-9	-1.22E-10	-7.43E-5	-0.0127	-0.113
Butene (co-product)	-0.0014	-1.02E-8	-0.582	-0.0001	-3.19	-0.530	-6.30E-9	-1.55E-9	-0.0001	-0.0191	-0.221
Ethane (co-product)	-0.0013	-5.46E-9	-0.501	-0.0003	-0.934	-0.118	-1.86E-8	-4.21E-8	-0.0002	-0.0064	-0.011
Propane (co-product)	-0.0003	-8.2E-10	-0.076	-7.71E-5	-0.311	-0.033	-3.42E-9	-3.48E-8	-2.88E-5	-0.0023	-0.010
Butane (co-product)	-0.0009	-3.70E-9	-0.340	-0.0002	-0.632	-0.081	-1.26E-8	-2.84E-8	-0.0001	-0.0044	-0.009
<i>Fossil-based BTX aromatics</i>											
TOTAL	0.0048	4.45E-8	2.18	0.0006	9.13	1.65	3.33E-8	1.42E-8	0.0004	0.066	1.28
<i>Standard deviation</i>	<i>9.50E-5</i>	<i>2.32E-8</i>	<i>2.52</i>	<i>0.00019</i>	<i>0.039</i>	<i>0.013</i>	<i>8.15E-8</i>	<i>7.16E-9</i>	<i>3.11E-5</i>	<i>0.0018</i>	<i>3.45</i>

Table S26. Life cycle assessment results for Case D – olefins-rich product in which pyrolysis of mixed plastic waste is used to produce ethylene under a high selectivity towards olefins scenario, related to **Fig. 7g-h** in the main text. The results for fossil-based ethylene are included for comparison.

	<i>Impact category</i>										
	Acidif-ication kg SO ₂ eq/kg	Carcin-ogenics CTUh/kg	Eco-toxicity CTUe/kg	Eutro-phication kg N eq/kg	Fossil fuel depletion MJ surplus/kg	Global warming kg CO ₂ eq./kg	Non carcin-ogenic CTUh/kg	Ozone depletion kg CFC- 11/kg	Particulates kg PM2.5 eq/kg	Smog kg O ₃ eq/kg	Water use m ³ /kg
<i>Case D: mixed plastic waste pyrolysis for ethylene</i>											
TOTAL	0.0193	3.04E-7	141	0.0527	-18.1	5.34	2.74E-6	8.53E-7	0.0122	0.138	37.1
Standard deviation	0.00525	5.20E-7	57.1	0.0221	2.03	0.475	1.28E-6	5.08E-7	0.00171	0.0243	59.5
Process Emissions	0	0	0	0	0	1.40	0	0	0	0.0000	0
Catalyst	5.84E-5	4.32E-10	0.057	3.69E-5	0.011	0.011	2.13E-9	1.32E-9	1.49E-5	0.0005	0.006
Cooling Water	3.05E-5	1.58E-9	0.115	2.59E-5	0.007	0.007	3.31E-9	6.23E-10	9.31E-6	0.0004	38.4
Process Water	2.37E-5	6.53E-10	0.037	1.75E-5	0.004	0.004	1.48E-9	1.67E-9	9.16E-6	0.0003	0.120
DMF	3.99E-5	2.75E-10	0.046	4.77E-5	0.021	0.006	1.77E-9	1.52E-9	7.14E-6	0.0003	0.004
Sulfolane	0.0001	2.32E-10	0.027	1.66E-5	0.022	0.004	1.05E-9	8.04E-10	1.20E-5	0.0002	0.008
Natural Gas	0.0041	5.79E-9	0.763	0.0002	2.38	0.122	2.90E-8	2.18E-7	0.0003	0.0068	0.008
Infrastructure	3.19E-7	1.07E-11	0.002	4.45E-7	2.71E-5	3.61E-5	9.5E-11	2.59E-12	7.55E-8	2.44E-6	9.7E-6
Steam	0.0103	3.90E-8	3.65	0.0024	5.03	2.68	1.62E-7	3.33E-7	0.0011	0.0787	0.140
Plastic feedstock	0.0121	1.75E-7	121	3.20E-2	4.99	3.53	2.03E-6	5.74E-7	0.00418	0.201	0.722
Electricity	0.0023	4.90E-8	5.59	0.0051	0.476	0.625	1.67E-7	6.64E-8	0.0020	0.0160	0.104
Refrigeration	0.0082	1.74E-7	19.9	0.0180	1.69	2.22	5.94E-7	2.36E-7	0.0070	0.0569	0.369
Solids Disposal	6.28E-6	6.47E-10	3.16	0.0002	0.001	0.014	4.23E-8	1.31E-10	9.87E-7	8.23E-5	0.000
Wastewater	3.83E-6	1.31E-10	0.010	2.43E-5	0.000	0.000	2.33E-9	3.28E-11	7.32E-7	3.76E-5	-0.031
Aromatics (co-product)	-0.0041	-4.88E-8	-4.86	-0.0033	-3.97	-1.05	-1.61E-7	-4.85E-8	-0.0010	-0.0487	-0.636
Naphtha (co-product)	-0.0030	-1.00E-8	-0.906	-0.0011	-4.56	-0.285	-3.75E-8	-5.17E-7	-0.0003	-0.0250	-0.147
BTX (co-product)	-0.0039	-3.65E-8	-1.78	-0.0005	-7.49	-1.35	-2.73E-8	-1.16E-8	-0.0004	-0.0537	-1.052
Propylene (co-product)	-0.0047	-2.98E-8	-1.64	-0.0003	-11.4	-1.70	-1.45E-8	-6.11E-10	-0.0004	-0.0639	-0.567
Butene (co-product)	-0.0023	-1.71E-8	-0.979	-0.0002	-5.36	-0.891	-1.06E-8	-2.61E-9	-0.0002	-0.0321	-0.372
<i>Fossil-based ethylene</i>											
TOTAL	0.0195	3.52E-8	4.70	0.0016	11.4	1.32	1.61E-7	1.20E-6	0.016	0.049	0.198
Standard deviation	4.16E-6	1.64E-8	1.28	5.97E-5	0.00044	0.0011	3.49E-8	1.54E-10	6.02E-7	3.00E-5	2.81

Materials and methods

Feedstock Pretreatment. The bales of mixed plastic feedstock are procured from a Materials Recovery Facility (MRF) where it is assumed to have gone through initial sorting, cleaning, removal of metals, etc. The size of the pyrolysis facility (240 TPD) is selected to be consistent with average size of local MRF's in the United States. For context, some of the largest MRFs in the U.S. have a plastic processing capacity of 500–600 TPD. In the U.S., fewer than 10% of MRFs (from a total of approximately 300 MRFs) have a processing capacity of over 500 TPD of plastics, while 66% of the MRFs have a throughput less than 300 TPD. Next, the mixed plastic bales are converted to flakes at an additional cost of \$0.42/kg at the pyrolysis facility.¹⁵ The processing of feedstock in the base case design begins with size reduction of the mixed waste plastic flakes by two sequentially arranged hammer mills requiring a power input of 110 kWh/MT.^{15, 16} The size of the feedstock is reduced up to 2–3 mm in diameter for maximizing heat transfer in the pyrolysis reactor associated with anisotropic properties of the feed. Any moisture in the feedstock is removed through a crossflow pellet dryer utilizing hot flue gases from the combustion reactor outlet. PVC decomposition in the pyrolysis reactor operation can lead to corrosion of process equipment, choking of downstream product separation trains, and release of environmental toxins.¹⁷ Thus, it is removed by thermal degradation of the polymer at 300°C to release chlorine in the form of hydrochloric acid.^{17, 18} The hot hydrochloric vapors are quenched with water and diluted to 30 wt% concentration before routing it to the wastewater treatment section. **Fig. 4** presents a simplified process flow diagram (PFD) for the base case, whereas detailed PFD indicating all model inputs and a full summary of stream compositions is provided in **Fig. S1**.

Design and Operation of CFP Reactor. An *in situ* system combines polymer deconstruction and catalytic upgrading of vapors within the same dual-stage, circulating, fluidized bed fast pyrolysis reactor systems. This has the potential to reduce capital costs by precluding the use of additional vapor phase upgrading reactors such as those in an *ex situ* configuration. The solids consisting of catalyst mixed with char and/or coke exit the riser reactor and are separated from the vapors in two cyclones connected in series (**Fig. S1**). The combustor also serves as a catalyst regenerator by burning off coke deposits. The combustor is operated at nearly the same pressure as the reactor. The reactor and combustor capital costs are scaled based on actual gas volumetric flow rate in our assessment. A fired heater is modelled to burn the process char and heavies, as well as some gaseous process intermediates in combustor, to provide sufficient heat to the *in situ* reactor. The hot stack gases generate high pressure steam (600 psig) in a boiler that in turn heats up the bed material, which is eventually fed into the *in situ* reactor. The temperature of combustor reactor is selected to be 720°C, based on constraints for operation of the ZSM-5 catalyst. The typical FCC replenishment rates are between 1% and 3% every day.¹² In this work, two percent of the catalyst inventory is replenished every day assuming an additional 1.6% of attrition rate. The catalyst is modeled as an olivine component in Aspen Plus and heated throughout the combustion process. A solids cooler is used in the combustor to partially cool the hot catalyst, allowing it to control the *in situ* reactor exit temperature of 670°C through the thermal capacity of the hot catalyst. Also, a steam stripper has been included in the reactor system to recover additional products (mainly coke deposits) from catalyst surface. Similar to Dutta *et al.*, a design specification of 1.36 kg of steam per 453.59 kg of catalyst was used.^{19, 20} The cost of an additional vessel was added for this purpose and was sized assuming a height of 28 feet. Recycled light gases are used as the carrier gas for entraining the catalyst and mixed plastics feed. The reactor was modeled such that the bed is in a fluidized state and the pressure drop across the bed does not exceed 3 bar. The catalyst to plastic feed ratio of 6 and high process temperature (670°C) employed in the base case design results in increased yields of both olefins (34.9 wt%) and total aromatic compounds (32.7 wt%).

Catalyst Selection for Catalytic Fast Pyrolysis with *in situ* Vapor Upgrading. The *in situ* configuration combines fast pyrolysis and catalytic vapor upgrading within the same reactor. Spent FCC catalyst was

used in combination with a ZSM-5 catalyst in the proportion 62.5 wt% spent catalyst and 37.5 wt% of ZSM-5.⁷ The spent FCC catalyst is modelled to be obtained from an operating refinery, with 0.23 wt% residual coke on its surface and a commercial ZSM-5 was modeled. The spent catalyst helps in maintaining the catalyst activity at a constant level without producing high levels of methane and coke.⁷ For context, fresh FCC catalysts have a very high surface area (roughly 50% or more) compared to spent FCC catalysts and, as a result, a high activity. High catalyst activity increases feed cracking, resulting in higher yields of coke or light gases such as methane, which is avoided in this study. The price of spent FCC catalyst (62.5 wt%) and ZSM-5 zeolite (37.5 wt%) used in this study was estimated to be \$2.98 per kg using the CatCost tool.¹⁴ Details on the catalyst cost estimation can be found in **Table S27**. A detailed PFD and a full summary of stream compositions are provided in **Fig. S1**.

Phase Separation and Products Recovery. The hot pyrolysis vapor effluent is routed to a three-stage quenching/condensation that lowers the temperature of hot vapor from 670°C to 25°C. Heat integration was employed to supply energy to the dechlorination reactor in the Feedstock Pretreatment section by utilizing the heat dissipated from cooling the hot vapors (670°C) in the Phase Separation section. Next, a flash vessel at 21°C separates a light gaseous stream (47 wt%) from the residual heavier liquid bottom (50 wt%). The yield of liquid product boiling at <220°C is 43.5 wt% and contains approximately 76 wt% aromatic compounds. The gaseous products, rich in olefinic gases, are sent to the olefins recovery process section for monomers (olefins) separation and the liquid from the bottoms is sent to the aromatic hydrocarbons recovery process section for the extraction and purification of aromatic products. Due to the specific catalytic activity of the spent FCC and ZSM-5 catalysts employed in this design, formation of methane and coke, as well as the formation of heavy liquid products (bp >370°C) is greatly suppressed. The process heavies are routed to the combustor of the CFP reactor system, where they are utilized as a fuel to heat the reactor. A portion of the non-condensable gases are recycled for use as fluidizing gas in the fast pyrolysis reactor. A detailed PFD and a full summary of stream compositions are provided in **Figure. S2**.

Olefin Separation and Recovery. Olefins recovery from the gaseous stream is modelled in three parts. *1) Upstream CO₂ removal:* The pyrolysis gaseous effluent may contain CO₂ and H₂S, depending on the cracking feedstock, thus an acid-gas removal step that eliminates all CO₂ and/or H₂S from the cracked gas is incorporated in the front-end section to remove CO₂ by absorption in a solvent upstream or before the gas enters the chilling train. The removal of CO₂ is important both from a fuel value standpoint (increasing heating value) and protection against downstream corrosion due to its acidic nature. There is a risk of CO₂-freeze at low temperature condition and may be damaging for the heat exchanger and fractionation equipment.²¹ Additionally, CO₂ can be absorbed into ethylene, affecting product quality and further processing.²² Thus, CO₂ was removed (below 0.2 ppm) by a rate-based model in Aspen Plus using monoethanolamine (MEA) as a solvent. A packed column was utilized for CO₂ absorption using a 30 wt% MEA solution, and the CO₂ was removed from the top of a desorber column while the lean solvent was recycled. A detailed PFD and a full summary of stream compositions are provided in **Fig. S3**.

2) Chilling train: The chilling train configuration was modelled after standard industrial separation processes in ethylene and propylene plants.²² The remainder of the light stream after CO₂ removal is pressurized to up to 37 bar (from 5 bar) and simultaneously cooled to 50°C by a system of five-stage compressors. During compression, the temperature of olefin-rich gaseous stream is maintained under 100°C by interstage cooling to prevent olefin polymerization and subsequent equipment fouling. Sequentially, the olefinic gases are further cooled and pre-separated in a series of cold boxes essentially comprising refrigeration coolers (Chiller-1 to Chiller-5), an expander (EXP), and knock out (KO) drums as shown in **Fig. S3**. Streams in the chilling train are cooled and reheated counter-currently throughout in plate-fin heat exchangers, which are also known as brazed aluminum heat exchangers (BAHX). Multiple, well-insulated

BAHX units are combined in a cold box, which sometimes also includes vessels or KO drums with a minimum temperature approach (MITA) of 3°C. Similar to an olefins plant, there are multiple liquid demethanizer feed streams (streams containing methane) coming out of the chilling train, at different temperatures and with different compositions, and they are fed to different locations in the demethanizer.²³

3) Downstream separation: Methane (1.5 wt%) and hydrogen (0.1 wt%) are removed from the top of demethanizer in the liquid phase. Note that the demethanizer is the coldest point in the separation train. Literature data from olefins plants served as the basis to set the separation sequence of the refinery.²³ Ethylene and propylene, or propane, are often used as refrigerants in older olefin plants. Newer plants often have binary or even tertiary refrigeration systems and sometimes also employ turbo-expanders. Separation of the C₁ to C₄ gases at low temperatures requires the use of refrigeration cycles as well as high pressure steam. Therefore, the designed refrigeration cycles are integrated to maintain low-temperature conditions, as well as to reduce the overall cooling utilities. Finally, the bottom product of the demethanizer is nearly methane-free and is introduced into a deethanizer column. The gas product (top) from the deethanizer is fed into a C₂ splitter for the separation of ethylene from ethane. The bottom product is fed to the depropanizer. The overhead product of the depropanizer is sent to a C₃ fractionator that requires 140 trays in the distillation column. Polymer-grade (>99.5% purity) ethylene and propylene are obtained from the top of columns C₂ and C₃ fractionators, respectively, whereas ethane and propane are recovered from the bottom of these columns. Lastly, a debutanizer is used to separate the bottom product received from the depropanizer into a C₄ mixture (butene = >75% and butane = >23%) and C₅₊ (**Fig. S3**).

Separation of 1-butene and 1,3-butadiene from Butane. Butane and butene are usually obtained by fractionating cuts comprising C₄- hydrocarbons from steam or naphtha crackers. Since the boiling points of butane (-1°C) and butene (-6.3°C) are very close, they form a minimum boiling azeotrope mixture, which is difficult to separate by normal distillation processes. Therefore, a third component – a separating agent, most commonly a polar solvent, is employed to alter the relative volatilities of the components to be separated. On an industrial scale, extractive distillations with polar solvents are usually carried out. For example, a patent describes the separation of a C₄ cut freed of butadiene by extractive distillation with N-methylpyrrolidone (NMP)²⁴ and another discloses the use of dimethylformamide (DMF) as a polar extractant for butene/butane separation.²⁵ Likewise, other solvents such as acetonitrile, furfural, N-formylmorpholine, or dimethylacetamide have been used either anhydrously or in a mixture with water.²⁴

Since recovering high-value products, especially 1-butene, is currently more profitable, an extractive distillation step was included to separate the C₄ mixture containing butane, 1-butene, and butadiene. DMF as a solvent was introduced from the top (6th stage) to flow counter-currently to the flow of feed (fed from stage 41). Due to the difference in boiling points of the polar extractant and the lower boiling aliphatic C₄ hydrocarbon, the butane is recovered from the top of the first column after the gaseous C₄ feed contacts the polar extractant with a mass ratio of 5.2:1. The top product, which is nearly 99% pure butane, is recovered, and the bottom product consisting of the butene/solvent mixture is introduced into a solvent recovery column. A reflux ratio of 1 enables complete separation of butene and butadiene as a low boiler fraction. Polymer-grade 1-butene is recovered from the top nearly free of the extractant, and the solvent recovered from the bottom is recycled back to the extractive distillation (ED) column (**Fig. S3**). The C₅₊ consisting mostly of naphtha components is sent to aromatics recovery process section and finally for the recovery of pyrolysis naphtha.

Aromatics Separation and Recovery. The main purpose of aromatic hydrocarbons recovery process section is the extraction of BTX aromatic hydrocarbons in a mixture that might be supplied directly to a benzene-toluene-xylenes (BTX) facilities or sold separately. The conceptual design of the extraction process is based on the sulfolane process designed by UoP Honeywell,²⁶ which has been adapted to the feed

composition estimated for the plastics CFP refinery studied here. The outstanding properties of sulfolane including selectivity to aromatics, miscibility in water, stability and a high boiling point make this solvent, the chosen solvent for the extractive distillation process. The aromatics containing streams coming from the Phase Separation and Olefins Recovery sections are mixed, and then pressurized and heated to 3.53 bar and 170°C.

The mixed feed is introduced from the bottom of the ED column and sulfolane is introduced at the top. The sulfolane removes around 66% of C₆–C₁₂ aromatic hydrocarbons using a solvent-to-feed ratio of 2 (mass basis).²⁷ Both the solvent and the feed are supplied at 170°C to improve the extraction. The distillate, rich in aliphatic hydrocarbons, is similar to naphtha. The bottoms, primarily containing aromatic compounds and sulfolane, are cooled down to 70°C and fed to a water wash column to remove aliphatic hydrocarbons with a carbon number greater than 12. Note that combining solvent with the feed alters the relative volatilities of the components in the feed because of the non-ideal behavior of the mixture, which is the key to the ED process. This extractor uses water at 90°C as a solvent, with a solvent-to-feed ratio of 0.06,²⁸ which clears almost 95% of heavy aliphatic hydrocarbons. The raffinate, which is rich in heavier hydrocarbons and containing some (<0.2%) solvent, is sent to the wastewater treatment. The extract is processed in a solvent recovery column (solvent stripper column). In this column, aromatic hydrocarbons are separated from the solvent under low vacuum (0.733 bar). Water is collected in the extract receiver boot and is directed to the water stripper. A detailed PFD and a full summary of stream compositions are provided in **Fig. S4**.

The distillate consists of a mixture of aromatics, traces of aliphatic hydrocarbons, and water, while the bottoms contain sulfolane (at 98.3% purity), which is recycled to the extractive distillation column. A two-phase separator reduces the water content of the distillate to yield a product with an aromatic content of 84%. Water from the bottoms of the separator is recycled to the wash column. The process requires make-up streams of sulfolane and water to maintain a constant solvent-to-feed ratio at the extractive distillation and wash columns, respectively. Finally, the BTX aromatic hydrocarbons are recovered from other aromatics (C₉–C₁₂) in a distillation column, and rest of the stream is recovered as a naphtha product.

Heat Integration. Heat integration was conducted for major process heating and cooling operations, such as heating of the dechlorination reactor and pyrolysis reactor, low-temperature cooling of gaseous olefin streams requiring refrigerants, and solvent recovery preheating. Specifically, heat leak into cold streams was considered a factor in the utilities operating expenses as it increases refrigeration requirements. Thus, heat leak for each BAHX was specified as percentage of duty.

Impact of Crude Oil Prices on the Economic Viability of Plastics Pyrolysis. Data from the Oil Price Information Service (OPIS) International Feedstocks Intelligence Reports for WTI (one of the crude oils used as a benchmark in oil pricing) range from \$30–\$120/bbl, and the prices of the specific year (15 years) served as the basis for the analysis product pricing structure. To capture the product pricing basis comprehensively, additional sources were included, mainly comprising S&P Global PLATTS, US Energy Information Administration (EIA) and IHS Markit.^{1, 10}

Property Methods and Property Estimation. Aspen Plus V10 was used for process modeling. Given the non-ideality of the components used in the simulation, the Poly-SRK property method was chosen for all CFP area unit operations. For olefins separation, the NRTL-RK property method was used, whereas UNIQUAC was specifically used for the extractive distillation column employed for the recovery of the aromatics fraction.

All pure component thermodynamic and physical properties were estimated using the National Institute of Science and Technology ThermoDataEngine (NIST-TDE) capabilities built into the Aspen Plus software

package. Binary interaction parameters were estimated using UNIFAC and fit to the NRTL-RK property method. The molecular weight of polymers was calculated based on the number of repeat units of each monomer comprising the polymer followed by the addition of repeat and end units.

Process Economics. Economic assumptions were consistent with other recent TEA modeling work,^{12, 15, 29} including cost year basis (2016), tax rate (21%), onstream time (90%), and plant startup time (0.5 years). For each process simulation, material, and energy flows calculated by the Aspen Plus process model were imported into an Excel spreadsheet, accounting for capital and operational costs. Given multiple products in the waste plastic processing facility, the selling price of BTX aromatic mixture was \$1.07 per kg based on the co-products revenues as determined using a DCFROR analysis to achieve a net present value (NPV) of zero assuming an after-tax rate of return of 10% over the 30-year lifespan of the refinery.

Capital Costs. All CFP area capital equipment base costs, scaling exponents, and installation factors were identical to that of the Dutta *et al.* report adjusted to a 2016 cost index.¹² In the olefins recovery and aromatics recovery section, the costs of pumps, compressors, distillation columns, and flash drums were calculated from the Aspen Capital Cost Evaluator (ACCE) V10 using flowrates and operating conditions imported from the results of the Aspen Plus simulation and standard refinery operating conditions^{22, 26} with default costing assumptions and a 2016 cost year.

While software and empirical correlations exist for sizing and costing standard equipment such as pumps, compressors, distillation columns, and common reactor types, novel reactor types typically lack these costing tools. To develop capital cost estimates for the CFP reactor, we used information provided by the Harris Group Inc., originally provided in Dutta *et al.*¹² These values were used as the cost basis in this work, with power law scaling using the actual volumetric flow rate. The reactor cost basis used from Dutta *et al.* was for biomass pyrolysis in an *in situ* reactor operating at 550°C temperature and 8 bar pressure.¹² All related TEA assumptions pertaining to installation factors, materials of construction, details of distillation columns e.g., number of plates, materials of construction, feed, and solvent introduction stages, operating and design pressures and temperatures etc. are included in **Table S7**.

Operating Costs. Variable operating costs for raw materials, wastes, utilities, and process byproducts were determined using flow rates from the Aspen Plus process simulation. While the economic analysis maintains a majority of cost assumptions used by Ward *et al.*,³⁰ several additions to downstream product separations were made to reflect actual refinery operations. Additional material costing assumptions, catalyst pricing methodology, and utilities calculation are summarized in **Table S4**, **Table S27**, and **Table S7**.

Catalyst cost estimates were generated using the CatCost tool assuming 455.5-ton order sizes (twice per year) and a 2016 cost basis (**Table S27**).¹⁴ Estimated delivered cost for mixed plastic waste feedstock varies depending on the sorting, MRF location, and the tipping fee. We assume here a delivered cost of \$0.18 per kg for the bales based on a US national average of mixed plastic streams from RecyclingMarkets.net⁸ and an additional \$0.42/kg for the flakes.

Supply Chain Energy and GHG emissions. Cradle-to-gate process inventories of the Case A – naphtha product, Case B – mixed product, Case C – aromatics-rich product, and Case D – olefins-rich product were adapted from the TEA models to be incorporated into the Materials Flows Through Industry (MFI) tool for supply chain analysis.³¹

Life Cycle Assessment: When available, United States-specific inventories from ecoinvent version 3.3 (allocation, cut-off by classification – unit) were utilized. If these data were unavailable, global inventories were used instead. ‘Allocation, cut-off by classification – unit’ refers to data in which recyclable products are available for use burden-free (i.e., no impacts associated with the original manufacture of those

products).³² Fossil-based BTX was approximated by a mixture of xylene (66%), toluene (30%), benzene (2.1%), and cumene (1.1%). The C₉–C₁₂ aromatic co-products were approximated by cumene. Data on the collection and sorting phases for HDPE and PP were obtained from the literature³³ and assumed to approximate inventories for a mixed plastic feedstock. The LCA was conducted with SimaPro 9.0 software using the TRACI 2.1 (US 2008) method;³⁴ water use was calculated by the AWARE method.³⁵ Solid waste (PVC and spent catalyst) was assumed to be landfilled. The system boundaries for MFI, LCA, and TEA are shown in Fig. S10. The uncertainties of background data were provided according to log-normal distributions in the ecoinvent database and Monte Carlo analysis was performed with 1,000 iterations to give standard deviation values.

Method for estimating cost of catalyst using CatCost model.

Table S27. Estimation of catalyst cost by CapEx & OpEx Factors method using the CatCost tool.¹⁴

CatCost v1.1.0 – 5 Outputs, CapEx & OpEx Factors Method		
Estimate: ZSM-5 37.5% with spent FCC catalyst		
<i>General Output Parameters</i>		
Unit Cost in Cents or Dollars (USD, \$)	Dollars	
Annual, Monthly, Weekly, Daily Cost?	Annual	
<i>Estimate Details</i>		
Basis Year	2016	
Design Production, Annual	8.26E+07	kg
Actual Production, Annual	8.26E+07	kg
<i>CapEx & OpEx Factors Outputs</i>		
<u>Cost Item</u>	<u>Unit Cost</u>	<u>Annual Cost</u>
	<u>\$/kg catalyst</u>	<u>\$/year</u>
<u>Capital Costs (10-year plant life)</u>		
Fixed Capital Investment	0.3385	27,977,448
Working Capital	0.0544	4,496,933
Total Capital Investment	0.3929	32,474,381
<u>Operating Costs</u>		
Direct Operating Costs		
Raw Materials	0.9736	80,465,962
Process Utilities	0.1503	12,423,225
Labor, Supplies, Maintenance, Lab	0.3368	27,831,039
Indirect Operating Costs		
Taxes, Insurance, Rent, Overhead	0.3181	26,290,936
General Expenses		
Admin, Dist., Mkting., R&D	0.3342	27,617,882
Total Operating Costs	2.1130	174,629,043
<u>Selling Margin</u>		
Return on Capital Investment (15%/yr of total capital invested)		
	0.5894	48,711,572
Flat Margin (disabled)	-	-
Total Margin	0.5894	48,711,572
Catalyst Purchase Cost	3.0954	255,814,995
Spent Catalyst Value (SCV)	0.1072	8,859,475
Net Catalyst Cost	2.9882	246,955,520

It was assumed that spent FCC catalyst is substituted for the clay binder normally used in the estimate for catalyst cost to make 25-50% ZSM-5. Therefore, rather than the \$0.11/kg for selling spent FCC catalyst to be used in cement applications, the price is assumed in the range of \$0.22–0.55/kg to account for the higher purity application.

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