Supplementary Information for:

Evaluation of Three Solvent-based Recycling Pathways for Circular Polypropylene

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S1. Base Case Equipment and Select Stream Details

The following sections provide more detailed information on the model results for each case. Both important stream information and process equipment sizing data are included.

S1.1. Solvent-Antisolvent Process

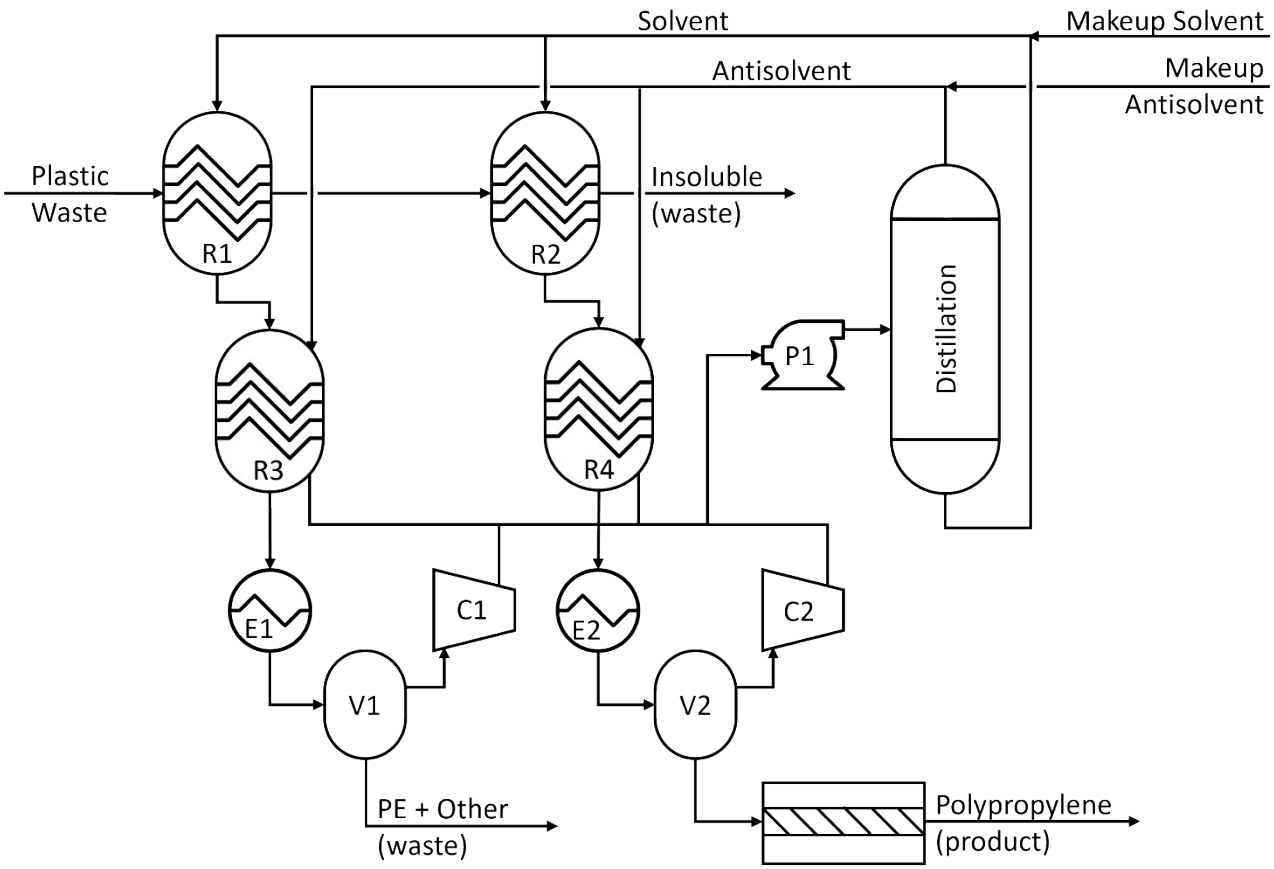

Figure S1. Simplified process flow diagram for the SA process. Process equipment (C for compressors, E for heat exchangers, P for pumps, R for heated semi-batch vessels, and V for vessels) is included in the following equipment table. Labeled streams are included in the following stream table. The Distillation column includes a column, feed preheater, reboiler, and condenser.

Table S1. SA process equipment list.

Compressors	Shaft Work (kW)	Inlet P. (kPa)	Outlet P. (kPa)
C1	5.6	2	101
C2	46.5	2	101
Column	**Diameter (m)**	**Height (m)**	
Column	2.7	4.9	
Pump	**Shaft Work (kW)**	**Outlet P. (kPa)**	
P1	0.5	111.5	
Heat Exchangers	**Area (m^2)**	**Duty (MJ/hr)**	**Fluid**
R1/R2 (3 vessels)	7.1	514~851	MP Steam
R3 (2 vessels)	24.8	2578	Cooling Water
R4 (2 vessels)	177.1	19588	Cooling Water
E1	0.6	213	HP Steam
E2	8.8	2364	HP Steam
Column Preheater	103.8	19691	LP Steam
Column Reboiler	189.0	25614	MP Steam
Column Condenser	156.5	24365	Cooling Water
C1 Interstage	0.4	80	Cooling Water
C2 Interstage	3.6	784	Cooling Water
Process Vessels	**Volume (m^3)**	**Pressure (kPa)**	
R1/R2 (3 vessels)	18.1	101	
R3 (2 vessels)	2.9	101	
R4 (2 vessels)	19.1	101	
V1	4.0	2	
V2	105.6	2	

Table S2. SA process abridged stream table.

Stream (Summary)	Units	Plastic Waste	Solvent	Antisolvent	Insoluble	PE + Other	PP Product	Makeup Solvent	Makeup Antisolvent
Phase		Solid	Liquid	Liquid	Wet Solid	Wet Solid	Solid	Liquid	Liquid
Total Mass Rate	kg/hr	5000	26682	62161	571	482	3977	26	5.1
Temperature	℃	25.0	132.9	69.6	140.0	163.9	214.8	25.0	25.0
Pressure	kPa	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Component Mass Rates	kg/hr								
XYLENE			26035	2281	19	2.1	4.7	26	5.1
HEXANE			643	59880	0.5	1.2	3.3		
POLYPROPYLENE		3950	4.0		3.0	3.9	3943		
POLYETHYLENE		500	0.5			475	25		
OTHER (PET)		550	0.0		549	0.5	0.5		

S1.2. Temperature Swing Process

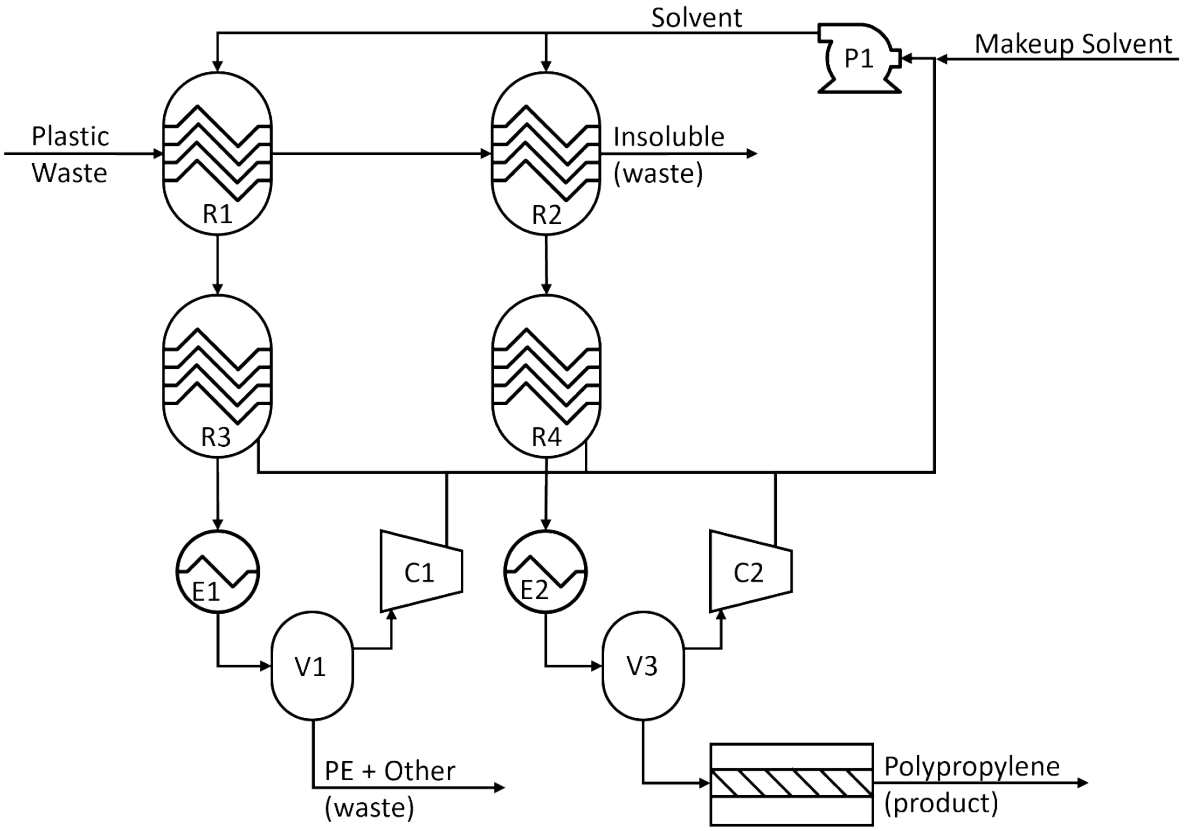

Figure S2. Simplified process flow diagram for TS process.

Table S3. TS process equipment list.

Compressors	Shaft Work (kW)	Inlet P. (kPa)	Outlet P. (kPa)
C1	28.7	2	101
C2	244.2	2	101
Pumps	**Shaft Work (kW)**	**Outlet P. (kPa)**	
P1	0.1	111	
Heat Exchangers	**Area (m^2)**	**Duty (MJ/hr)**	**Fluid**
R1/R2 (3 vessels)	20.4	1076~3994	MP Steam
R3 (2 vessels)	5.2	509	Cooling Water
R4 (2 vessels)	43.9	5771	Cooling Water
E1	1.4	483	HP Steam
E2	23.8	5638	HP Steam
C1 Interstage	1.3	330	Cooling Water
C2 Interstage	12.7	3625	Cooling Water
Process Vessels	**Volume (m^3)**	**Pressure (kPa)**	
R1/R2 (3 vessels)	17.7	101	
R3 (2 vessels)	0.7	101	
R4 (2 vessels)	5.2	101	
V1	97.6	2	
V2	29.6	2	

Table S4. TS process abridged stream table.

Stream (Summary)	Units	Plastic Waste	Solvent	Insoluble	PE + Other	PP Product	Makeup Solvent
Phase		Solid	Liquid	Wet Solid	Wet Solid	Solid	Liquid
Total Mass Rate	kg/hr	5000	26039	571	499	3988	58
Temperature	°C	25.0	60.3	140.0	128.0	208.5	25.0
Pressure	bar	1.0	1.0	1.0	1.0	1.0	1.0
Component Mas Rates	kg/hr						
XYLENE			26035	19	20	19	58
POLYPROPYLENE		3950	4.0	3.0	3.9	3943	
POLYETHYLENE		500	0.5	0.0	475	25	
OTHER (PET)		550	0.0	549	0.5	0.5	

S1.3. Supercritical Solvent Process

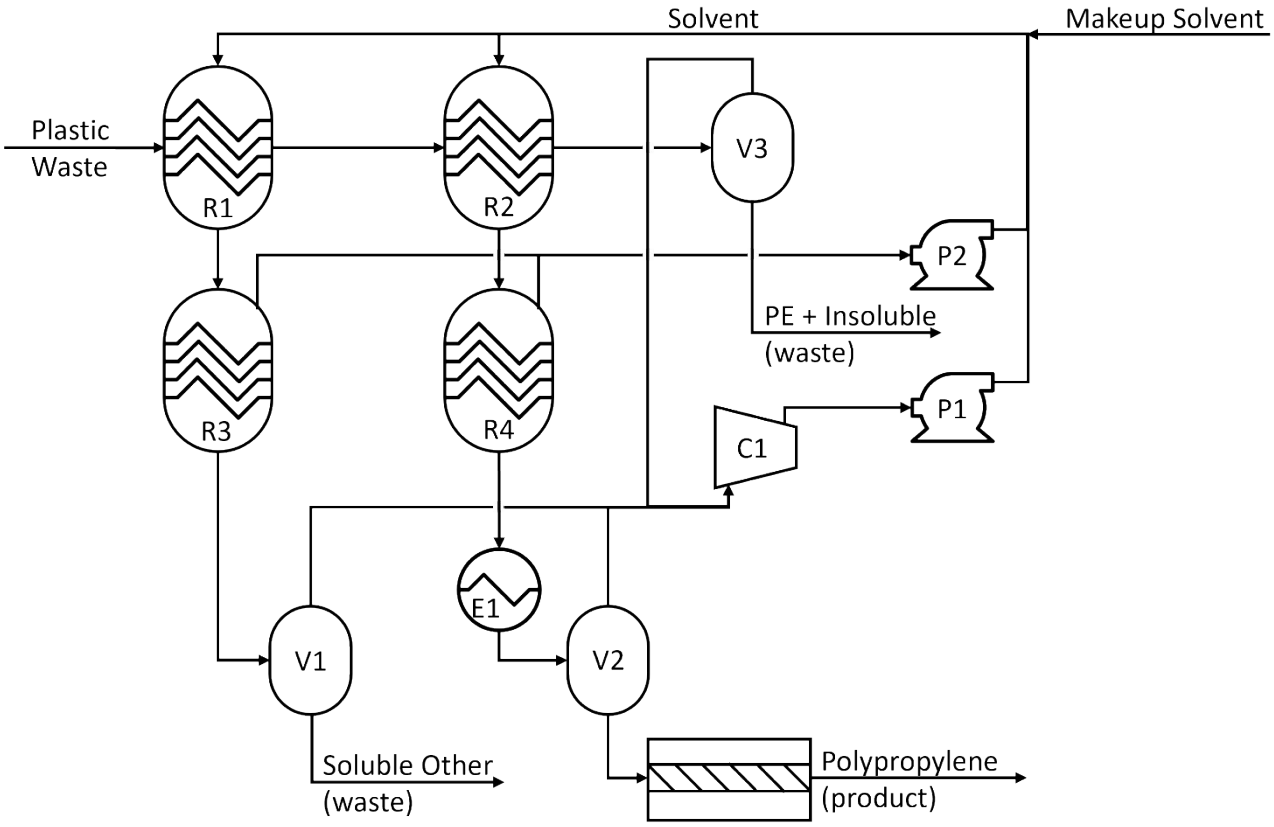

Figure S3. Process flow diagram for SS process.

Table S5. SS process equipment list.

Compressors	Shaft Work (kW)	Inlet P. (kPa)	Outlet P. (kPa)
C1	117.1	101	4000
Pumps	**Shaft Work (kW)**	**Inlet P. (kPa)**	**Outlet P. (kPa)**
P1	29.5	4000	25000
P2	188.5	20000	25000
Makeup Pump	0.2	1200	25000
Heat Exchangers	**Area (m^2)**	**Duty (MJ/hr)**	**Fluid**
R1/R2 (3 vessels)	10.9	411~1476	MP Steam
R3 (2 vessels)	0.8	165	Cooling Water
R4 (2 vessels)	5.6	1786	Cooling Water
E1	5.0	1217	HP Steam
C1 Interstage	3.2	688	Cooling Water

Vessels	Volume (m^3)	Pressure (kPa)
R1/R2 (3 vessels)	26.6	25000
R3 (2 vessels)	1.3	20000
R4 (2 vessels)	8.8	20000
V1	0.1	101
V2	0.2	101
V3	0.1	101

Table S6. SS process abridged stream tables.

Stream (Summary)	**Units**	**Plastic Waste**	**Solvent**	**PE + Insoluble**	**Soluble Other**	**PP Product**	**Makeup Solvent**
Phase		Solid	SC Fluid	Solid	Solid	Solid	SC Fluid
Total Mass Rate	kg/hr	5000	23650	504	527	3978	10
Temperature	°C	25.0	116.5	134.5	49.9	221.0	48.1
Pressure	bar	1.0	250.0	1.0	1.0	1.0	250.0
Component Mass Rates	kg/hr						
PROPANE			23646	0.5	6.3	3.5	10
POLYPROPYLENE		3950	3.9	5.1	3.9	3941	
POLYETHYLENE		500	0.0	499	0.5	0.5	
OTHER (PET)		550	0.6	0.0	517	33	

S2. Calculations for Process Economics

The process for calculating NPV, along with intermediate economic indicators such as capital cost and cash flow, is described by Turton et al.[1] The NPV in project year n, NPV_n, can be calculated from the sum of discounted cash flows:

$$NPV_n = -C_{TM} + \sum_{i=1}^{n} \frac{ATP}{(1-r)^n} \quad \text{(S1)}$$

where C_{TM} is the total module cost, or capital expenses (CAPEX), ATP is the annual after-tax profit, and r is the internal rate of return. The total module cost is the sum of the bare module cost, C_{BM}, of all pieces of equipment, p, multiplied by a factor that accounts for contingency and fees.:

$$C_{TM} = 1.18 \sum_{i=1}^{p} C_{BM,i} \quad \text{(S2)}$$

The total module costs are assumed to be invested in the three years leading up to the start of plant operation. Beginning in year 1, the annual after-tax profit is:

$$ATP = (R - COM - d_k)(1-t) + d_k \quad \text{(S3)}$$

where R is revenue from the sales of products (PP, waste plastic), COM is the cost of manufacturing, d_k is depreciation, and t is the effective tax rate.

The annual cost of manufacturing, COM, is calculated with the equation:

$$COM = 0.18C_{TM} + 2.73C_{OL} + 1.23(C_{RM} + C_{UT} + C_{WT}) \quad \text{(S4)}$$

where C_{OL} is the cost of operating labor, C_{RM} is the cost of raw materials, C_{UT} is the cost of utilities, and C_{WT} is the cost of waste treatment. C_{RM}, C_{UT}, and C_{WT} are based on the material balance and the prices of raw materials and utilities discussed in Section 2.3. The cost of operating labor is based on the number of pieces of major process equipment and solids handling sections. Depreciation is calculated linearly over the first five years of operation and a negligible salvage value is assumed.

References

[1] R. Turton, R. C. Bailie, W. B. Whiting, J. A. Sheaiwitz, D. Bhattacharyya, *Analysis, Synthesis, and Design of Chemical Processes*, Fourth ed., Prentice Hall, Tokyo, **2012**.