Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

High-purity Polypropylene from Disposable Face Masks via Solvent-Targeted Recovery and Precipitation

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Supporting information includes:

- Figure S1. (a) PP recovery yields and (b) undissolved solid residue yields at different temperatures for new and used masks. All experiments were operated for 5 mins.
- Figure S2. Overall yields based on different dissolution time conditions for new and used masks. All experiments were operated at 110°C.
- Figure S3. ATR-FTIR spectra of the STRAP residue at different dissolution time conditions from (a) new mask and (b) used mask.
- Figure S4. (a) ^{1}H NMR spectra and (b) ^{13}C NMR spectra of virgin PP and decolored PP in 1,1,2,2-tetrachloroethane-d_2.
- Table S1. Yields of STRAP residue from new and used mask.
- Table S2. Detailed color quantification results for ground PP without and with decolorization process, using virgin PP as a control sample (70 µm films). Each sample was tested for 4 times.

Economic impacts of the STRAP process including color removal:

- Figure S5. ATR-FTIR spectra of (a) fresh toluene and recycled toluene from stream No.13 and (b) fresh DMAc and distilled DMAc from stream No.26.
- Figure S6. HPLC analysis of (a) fresh toluene, (b) and recycled toluene from stream No.13, (c) fresh DMAc, and (d) distilled DMAc from stream No.26.
- Figure S7. GC-MS spectra of (a) fresh toluene and recycled toluene from stream No.13 and (b) fresh DMAc and distilled DMAc from stream No.26.
- Figure S8. Process flow diagram for the recovery of decolored PP in face masks using the STRAP technology. The numbers in each line denote the stream number.
- Table S3. General parameters for the technoeconomic analysis.
- Table S4. Installed equipment cost for a 5,292 ton/year plant to produce decolored PP from face masks.

- Table S5. Capital cost (CAPEX) for a 5,292 ton/year plant to produce decolored PP from face masks.
- Table S6. Fixed operating cost for a 5,292 ton/year plant to produce decolored PP from face masks.
- Table S7. Variable operating costs for a 5,292 ton/year plant to produce decolored PP from face masks.
- Table S8. Revenue for a 5,292 ton/year plant to produce decolored PP from face masks.
- Table S9. Stream list and mass balance for a 5,292 ton/year decolored PP plant.

Economic and environmental impacts of the STRAP process without color removal:

- Figure S9. Process flow diagram for the recovery of colored PP in face masks using the STRAP technology (without color removal process).
- Figure S10. Sensitivity analysis for important parameters of the process without color removal.
- Figure S11. Sensitivity analysis for economies of scale of the STRAP process without color removal.
- Figure S12. Climate change impact of producing colored PP via the STRAP process in comparison with virgin PP.
- Table S10. Installed equipment cost for a 5,292 ton/year plant to produce colored PP from face masks.
- Table S11. Capital cost (CAPEX) for a 5,292 ton/year plant to produce colored PP from face masks.
- Table S12. Fixed operating cost for a 5,292 ton/year plant to produce colored PP from face masks.
- Table S13. Variable operating costs for a 5,292 ton/year plant to produce colored PP from face masks.
- Table S14. Revenue for a 5,292 ton/year plant to produce colored PP from face masks. We assume that the selling price will be lower than the price of the decolored PP.

References

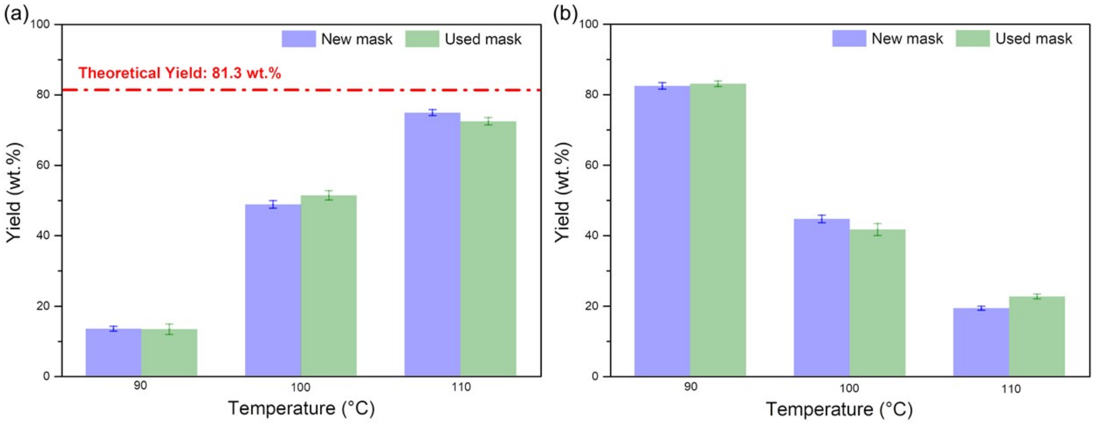

Figure S1. (a) PP recovery yields and (b) undissolved solid residue yields at different temperatures for new and used masks. All experiments were operated for 5 mins.

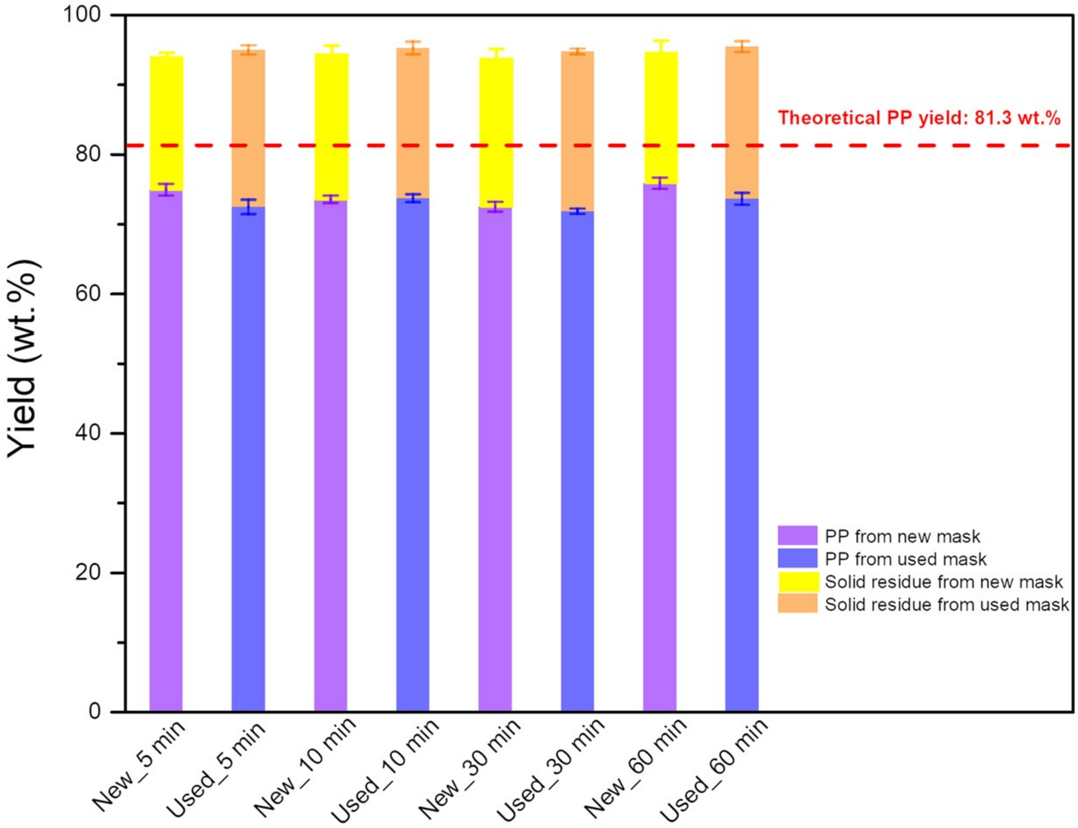

Figure S2. Overall yields based on different dissolution time conditions for new and used masks. All experiments were operated at 110°C.

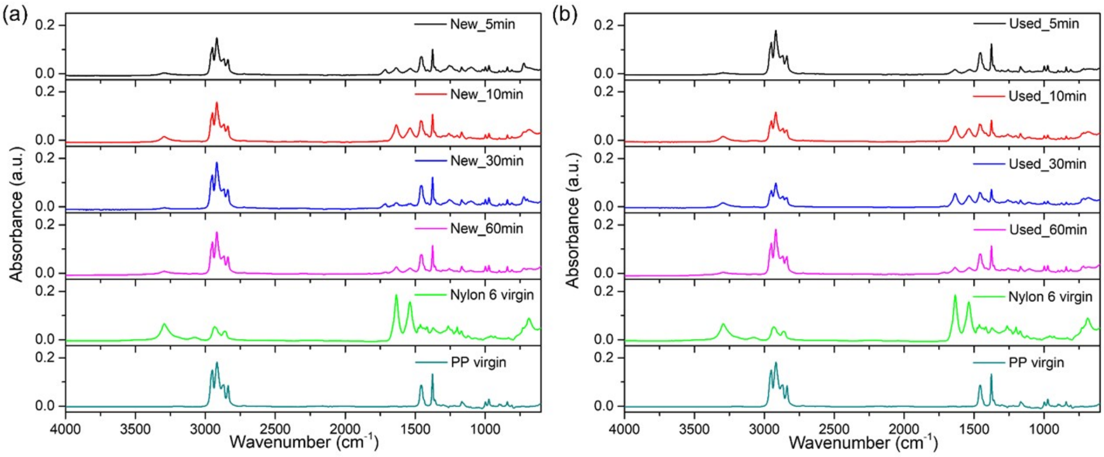

Figure S3. ATR-FTIR spectra of the STRAP residue at different dissolution time conditions from (a) new mask and (b) used mask.

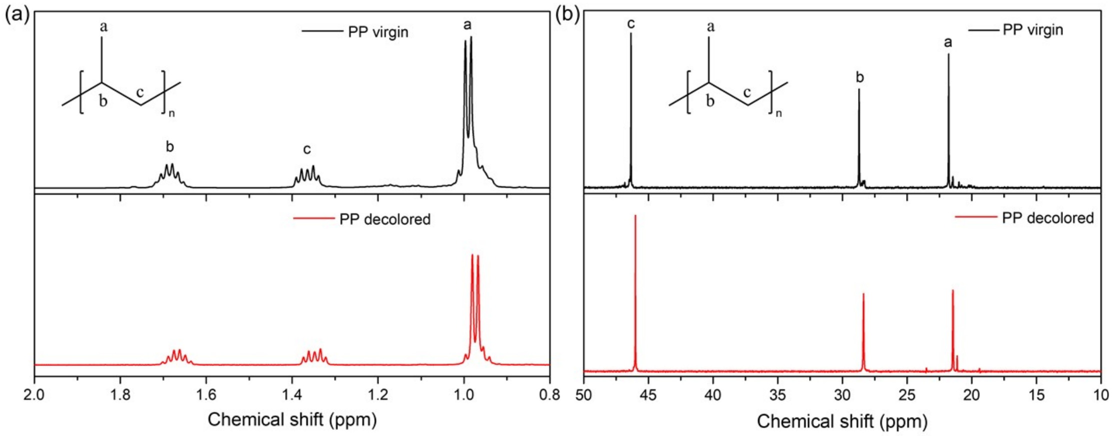

Figure S4. (a) ^{1}H NMR spectra and (b) ^{13}C NMR spectra of virgin PP and decolored PP in 1,1,2,2-tetrachloroethane-d_2.

Table S1. Yields of STRAP residue from new and used mask.

Dissolution time (min)	New mask STRAP residue yield (%)	Used mask STRAP residue yield (%)
5	19.23 ± 0.55 [a]	22.56 ± 0.67 [a]
10	21.06 ± 1.11 [a]	21.57 ± 0.91 [a]
30	21.45 ± 1.32 [a]	22.94 ± 0.39 [a]
60	18.94 ± 1.59 [a]	21.87 ± 0.77 [a]

Same letter in the same column indicates statistical insignificance by Duncan's multiple range test.

Table S2. Detailed color quantification results for ground PP without and with decolorization process, using virgin PP as a control sample (70 µm films). Each sample was tested for 4 times.

Name	**Number**	**Perceived lightness**	**Red/green balance**	**Yellow/blue balance**	**Yellowness Index**
		L*	**a***	**b***	**YI**
Virgin PP	1	95.93	1.75	-6.7	-11.19
	2	96.38	1.90	-7.34	-12.22
	3	96.18	1.84	-7.15	-11.94
	4	96.36	1.84	-7.12	-11.85
Ground PP_colored	1	86.83	-3.33	-8.15	-19.54
	2	89.41	-1.97	-7.75	-17.08
	3	89.40	-1.94	-7.75	-17.06
	4	89.16	-2.33	-8.10	-18.12
Ground PP_decolored_5min	1	92.20	0.65	-5.03	-9.25
	2	91.00	0.45	-4.15	-7.82
	3	91.05	0.27	-4.57	-8.78
	4	92.22	0.78	-4.72	-8.56
Ground PP_decolored_60min	1	92.22	0.83	-4.62	-8.32
	2	91.94	0.78	-4.14	-7.45
	3	92.33	0.93	-4.44	-7.89
	4	92.11	0.88	-4.22	-7.51

L* ≡ Perceived lightness (perfect black = 0; perfect white = 100)

a* ≡ Red/green balance; a* > 0 (red ↑); a* = 0 (gray); a* < 0 (green ↑)

b* ≡ Yellow/blue balance; b* > 0 (yellow ↑); a* = 0 (gray); b* < 0 (blue ↑)

YI ≡ Yellowness Index (as YI ↑, yellowness ↑)

Economic impacts of the STRAP process including color removal

Table S3. General parameters for the technoeconomic analysis.[1, 2]

Parameter	Value
Lifetime (years)	20
Interest rate (%)	10
Income tax rate (%)	25
Depreciation method	MACRS
Plant operability per year (hours)	8,000
Lang factor	3.63
ISBL costs	Lang Factor multiplied by the equipment purchase cost
Chemical Engineering Plant Cost Index	776.9

Table S4. Installed equipment cost for a 5,292 ton/year plant to produce decolored PP from face masks.[3]

Equipment	Installed Cost (USD)
Shredder	232,582
Tanks	1,924,927
Vessels	249,969
Filters	2,982,158
Pumps	139,341
Extruder	6,292,230
Heat Exchangers	483,283
Dryers	5,571,297
Distillation column	313,427
Grinder	196,025
Total installed equipment costs	**18,385,240**

Table S5. Capital cost (CAPEX) for a 5,292 ton/year plant to produce decolored PP from face masks.

Category	Cost (USD)
ISBL costs (total installed equipment costs)	18,385,240
OSBL costs (30% of ISBL)	5,515,572
Engineering cost (15% of the ISBL plus OSBL)	3,585,122
Contingency cost (20% of the ISBL plus OSBL)	4,780,162
Total capital cost	**32,266,096**

Table S6. Fixed operating cost for a 5,292 ton/year plant to produce decolored PP from face masks.

Category	Cost (USD/year)
Operator salaries	208,050
Benefits and overhead (50% of salary)	104,025
Maintenance (3% of CAPEX)	967,983
Insurance (0.7% of CAPEX)	225,863
Total fixed operating costs	**1,505,921**

Table S7. Variable operating costs for a 5,292 ton/year plant to produce decolored PP from face masks.

Category	Unitary cost	Cost (USD/year)
Electricity	0.07 USD/kWh	360,160
Natural gas	0.016 USD/kWh	181,524
Low-pressure steam	1.79×10^{-6} USD/kJ	20,960
Medium-pressure steam	2.32×10^{-6} USD/kJ	9,120
Cooling water	3.43×10^{-7} USD/kJ	1,040
Cooling agent (chilled water)	5×10^{-6} USD/kJ	153,440
Cooling agent (chilled brine)	8.15×10^{-6} USD/kJ	134,080
Cooling agent (propane)	1.32×10^{-5} USD/kJ	37,120

Toluene (99.97% of recovery)	0.85 USD/kg	19,194
DMAc (99.98% of recovery)	2.55 USD/kg	30,568
Total variable operating costs		**947,206**

Table S8. Revenue for a 5,292 ton/year plant to produce decolored PP from face masks.

PP production (kg/year)	Selling price (USD/kg)[4]	Revenue (USD/year)
3,952,160	2.52	9,959,443
Total revenue		**9,959,443**

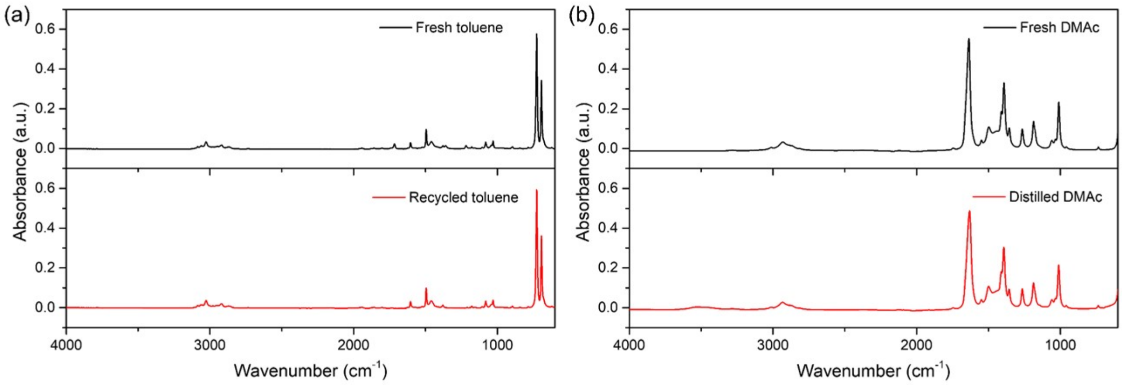

Figure S5. ATR-FTIR spectra of (a) fresh toluene and recycled toluene from stream No.13 and (b) fresh DMAc and distilled DMAc from stream No.26.

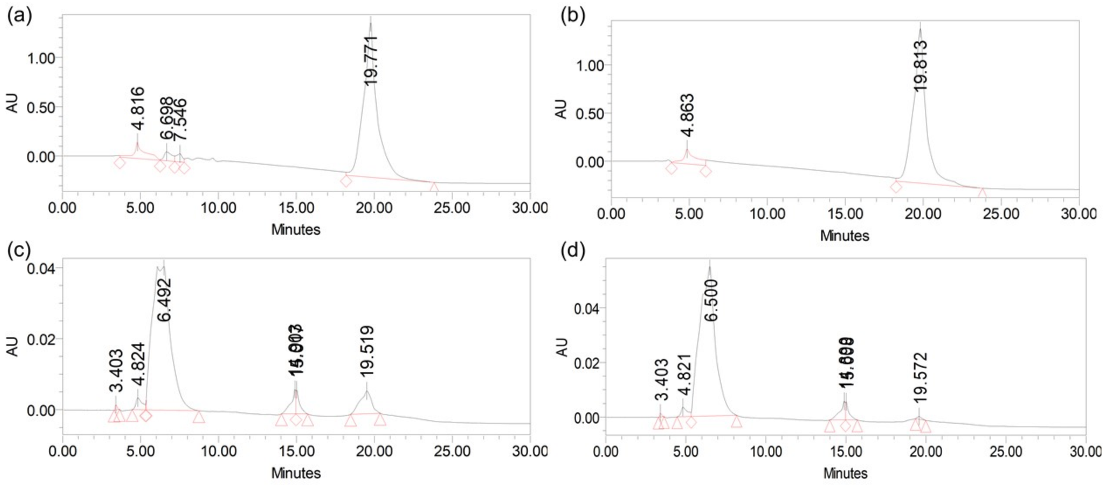

Figure S6. HPLC analysis of (a) fresh toluene, (b) and recycled toluene from stream No.13, (c) fresh DMAc, and (d) distilled DMAc from stream No.26.

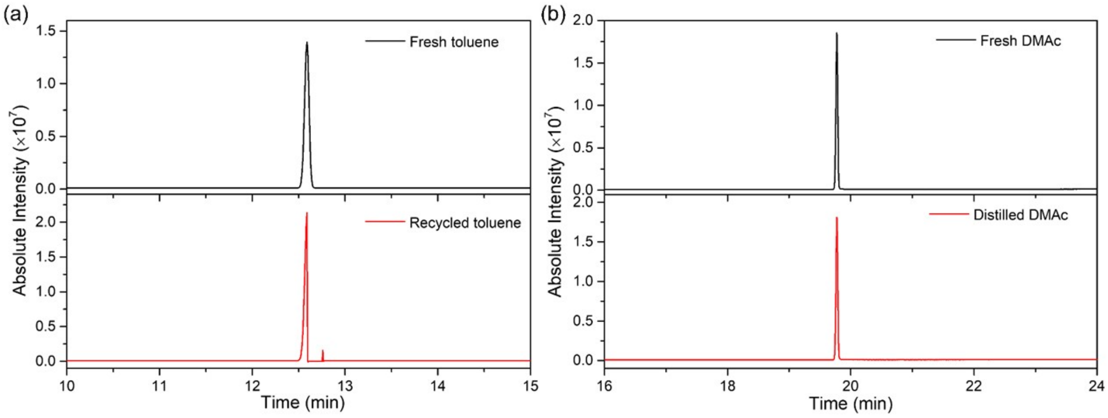

Figure S7. GC-MS spectra of (a) fresh toluene and recycled toluene from stream No.13 and (b) fresh DMAc and distilled DMAc from stream No.26.

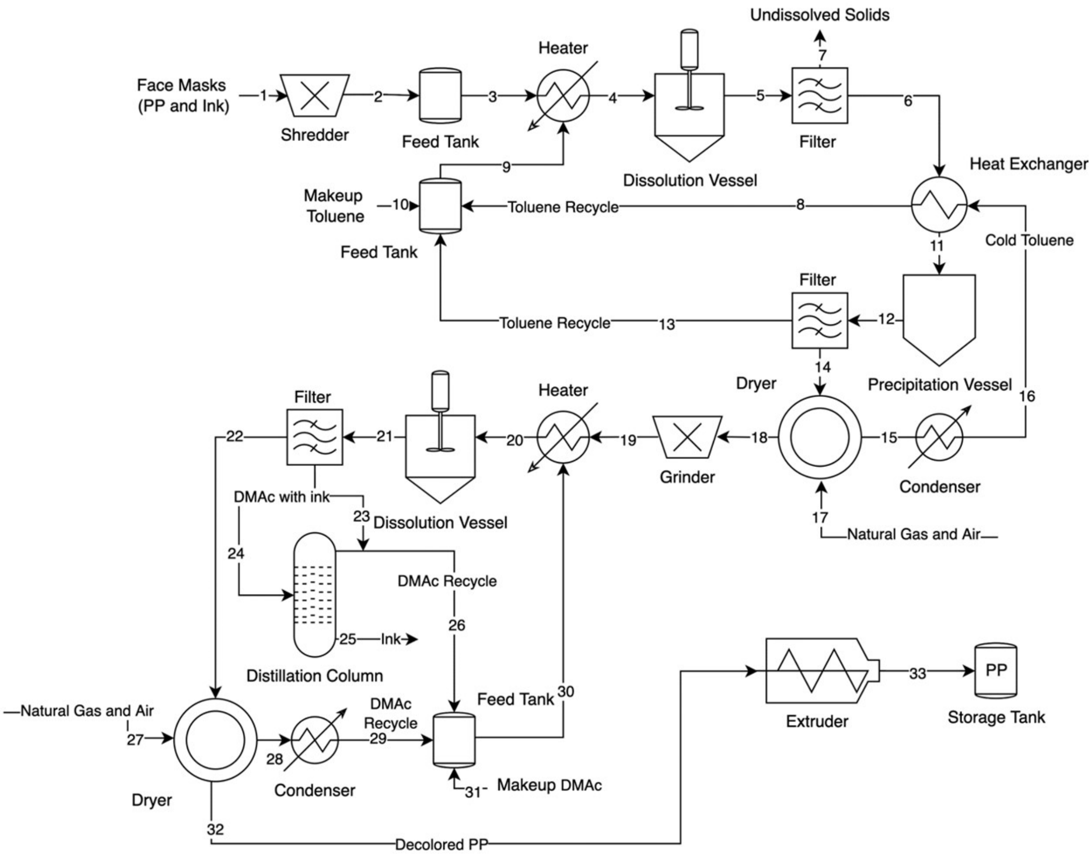

Figure S8. Process flow diagram for the recovery of decolored PP in face masks using the STRAP technology. The numbers in each line denote the stream number.

Table S9. Stream list and mass balance for a 5,292 ton/year decolored PP plant.

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Temperature (°C)	25	25	25	110	110	110	110
Component Flow Rate (kg/hr)							
Face masks (PP and ink)	662	662	662	662	662	496	0
Toluene	0	0	0	9923	9923	9923	0
Undissolved solids	0	0	0	0	0	0	166
Stream Number	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Temperature (°C)	68	25	25	60	60	60	60
Component Flow Rate (kg/hr)							
Face masks (PP and ink)	0	0	0	496	496	0	496
Toluene	5575	9923	2	9923	9923	4346	5577
Stream Number	**15**	**16**	**17**	**18**	**19**	**20**	**21**
Temperature (°C)	110.6	-37	25	110.6	110.6	115	115
Component Flow Rate (kg/hr)							
Face masks (PP and ink)	0	0	0	496	496	496	496
Toluene	5577	5575	0	0	0	0	0
DMAc	0	0	0	0	0	7443	7443
Natural gas	0	0	76	0	0	0	0
Stream Number	**22**	**23**	**24**	**25**	**26**	**27**	**28**
Temperature (°C)	115	115	115	151	90	25	165
Component Flow Rate (kg/hr)							
PP	494	0	0	0	0	0	0
Ink	0	1.8	0.2	0.2	1.8	0	0
DMAc	1489	5359	595	1	5953	0	1489
Natural gas	0	0	0	0	0	28	0
Stream Number	**29**	**30**	**31**	**32**	**33**		
Temperature (°C)	-37	90	25	165	165		
Component Flow Rate (kg/hr)							
PP	0	0	0	494	494		

Ink	0	1.8	0	0	0
DMAc	1489	7443	1	0	0
Natural gas	0	0	0	0	0

<u>Economic and environmental impacts of the STRAP process without color removal</u>

Technoeconomic Analysis

We performed a technoeconomic analysis (TEA) based on the collected experimental data of the process without the color removal to analyze its economic feasibility. Figure S9 shows the process flow diagram indicating the main equipment units and the input (face masks and toluene) and output (colored polypropylene) streams. Here, we can see the general steps of the process. First, the face masks are shredded and the stream together with the toluene stream are heated and mixed in the dissolution vessel. This mixture is filtered and cooled down before fed to the precipitation vessel. After this vessel, the mixture is filtered again. The liquid toluene stream is recycled and the other stream with polypropylene (PP) and toluene is dried to finally have a solid stream of PP and a gas stream of toluene. The toluene stream is condensed, and the resulting liquid stream of cold toluene is used as a cooling agent in the heat exchanger to reduce utilities costs; after, this toluene stream is also recycled. The solid PP stream is sent to the extruder and storage tank.

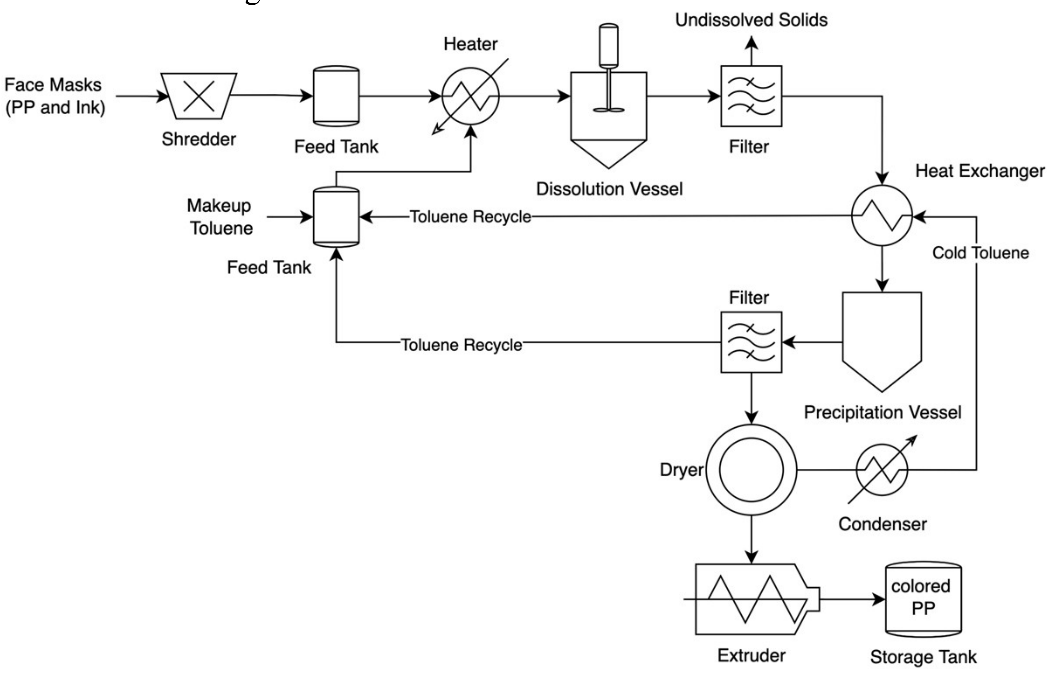

Figure S9. Process flow diagram for the recovery of colored PP in face masks using the STRAP technology (without color removal process).

Mass and energy balances were used to estimate the capital and operating costs of the process. We calculated the minimum selling price (MSP) of the PP for a plant capacity of 5,292 tons per year. We performed the process design and TEA using the open-source platform BioSTEAM. We consider 99.97% of solvent recovery for the toluene.

Other assumptions can be found in the Table S3. For the processing capacity of 5,292 tons per year, we found that the MSP of the colored PP was 1.42 USD/kg. This price is comparable to the average market values of virgin PP and the price of post-consumer PP (0.94-2.52 USD/kg).[4, 5] The total capital investment was 24.7 million USD, and the operating cost was 1.87 million USD per year. The detailed capital and operating costs are reported in the following Tables.

Table S10. Installed equipment cost for a 5,292 ton/year plant to produce colored PP from face masks.[3]

Equipment	Installed Cost (USD)
Shredder	232,582
Tanks	1,367,924
Vessels	186,492
Filters	2,018,891
Pumps	104,802
Extruder	6,307,385
Heat Exchangers	354,697
Dryers	3,504,888
Total installed equipment costs	**14,077,661**

Table S11. Capital cost (CAPEX) for a 5,292 ton/year plant to produce colored PP from face masks.

Category	Cost (USD)
ISBL costs (total installed equipment costs)	14,077,661
OSBL costs (30% of ISBL)	4,223,298
Engineering cost (15% of the ISBL plus OSBL)	2,745,144
Contingency cost (20% of the ISBL plus OSBL)	3,660,192
Total capital cost	**24,706,295**

Table S12. Fixed operating cost for a 5,292 ton/year plant to produce colored PP from face masks.

Category	**Cost (USD/year)**
Operator salaries	208,050
Benefits and overhead (50% of salary)	104,025
Maintenance (3% of CAPEX)	741,189
Insurance (0.7% of CAPEX)	172,944
Total fixed operating costs	**1,226,208**

Table S13. Variable operating costs for a 5,292 ton/year plant to produce colored PP from face masks.

Category	**Unitary cost**	**Cost (USD/year)**
Electricity	0.07 USD/kWh	259,360
Natural gas	0.016 USD/kWh	133,388
Low-pressure steam	1.79×10^{-6} USD/kJ	15,440
Cooling agent (chilled water)	5×10^{-6} USD/kJ	153,440
Cooling agent (chilled brine)	8.15×10^{-6} USD/kJ	30,000
Cooling agent (propane)	1.32×10^{-5} USD/kJ	37,120
Toluene (99.97% of recovery)	0.85 USD/kg	19,194
Total variable operating costs		**647,942**

Table S14. Revenue for a 5,292 ton/year plant to produce colored PP from face masks. We assume that the selling price will be lower than the price of the decolored PP.

PP production (kg/year)	**Selling price (USD/kg)[4]**	**Revenue (USD/year)**
3,952,160	1.50	5,928,240
Total revenue		**5,928,240**

The sensitivity analysis for selected parameters is presented in Figure S10. We estimated the MSP when the value of these parameters increases or decreases by 30%. We can see that the MSP is sensitive to the interest rate.

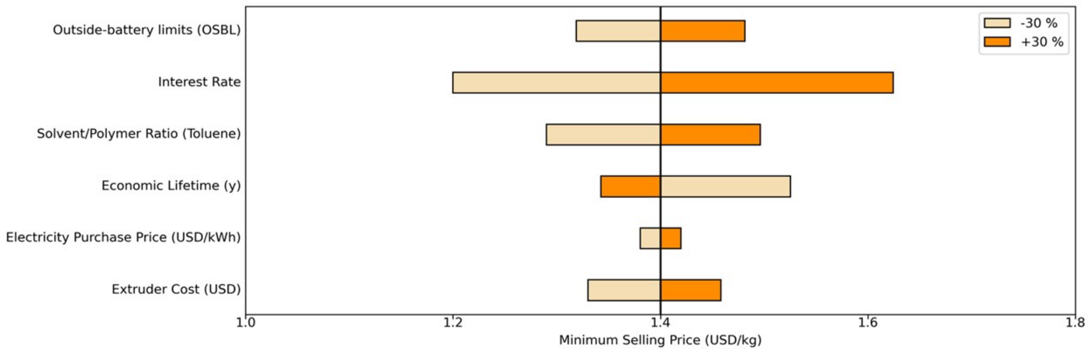

Figure S10. Sensitivity analysis for important parameters of the process without color removal.

The sensitivity analysis for different processing capacities to evaluate the impact of the economies of scale on the process is presented in Figure S11. We observe that after 7,000 tons per year, the MSP of the PP produced in the STRAP process is around half the maximum market value of the virgin resin and the price of post-consumer PP (0.94-2.52 USD/kg).[4, 5] These results demonstrate that the STRAP process without color removal is economically feasible, and that this technology could be installed at a large scale to recover the PP of the facemasks waste.

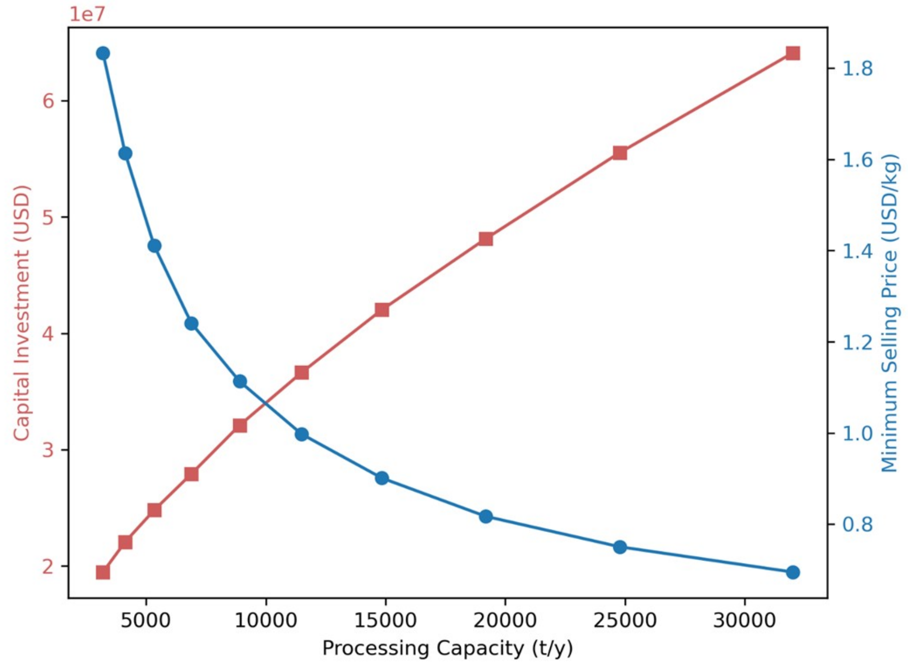

Figure S11. Sensitivity analysis for economies of scale of the STRAP process without color removal.

Environmental impact analysis

We analyzed the environmental impacts of the STRAP process without color removal using a life cycle assessment methodology and a product perspective (similarly to the environmental analysis that includes color removal). The functional unit considered is the production of 1 kg of PP. Therefore, we compare the environmental impacts of producing 1 kg of PP from traditional pathways with producing 1 kg of PP through the STRAP process. In Figure S12, we can see that the total impacts of the STRAP process without color removal (0.57 kg CO_2 eq./kg PP) are lower than the impacts of the virgin resin production (2.07 kg CO_2 eq./kg PP). Specifically, around 72% less emissions are generated in the STRAP process. The LCA data for solvents and for the virgin production of polypropylene are taken from the Ecoinvent 3.6 cut-off by classification database using the Environmental Footprint method. Data for the STRAP process utilities (steam, electricity, and cooling agents), as well as the transportation of commodities, are taken from the Environmental Footprint database.

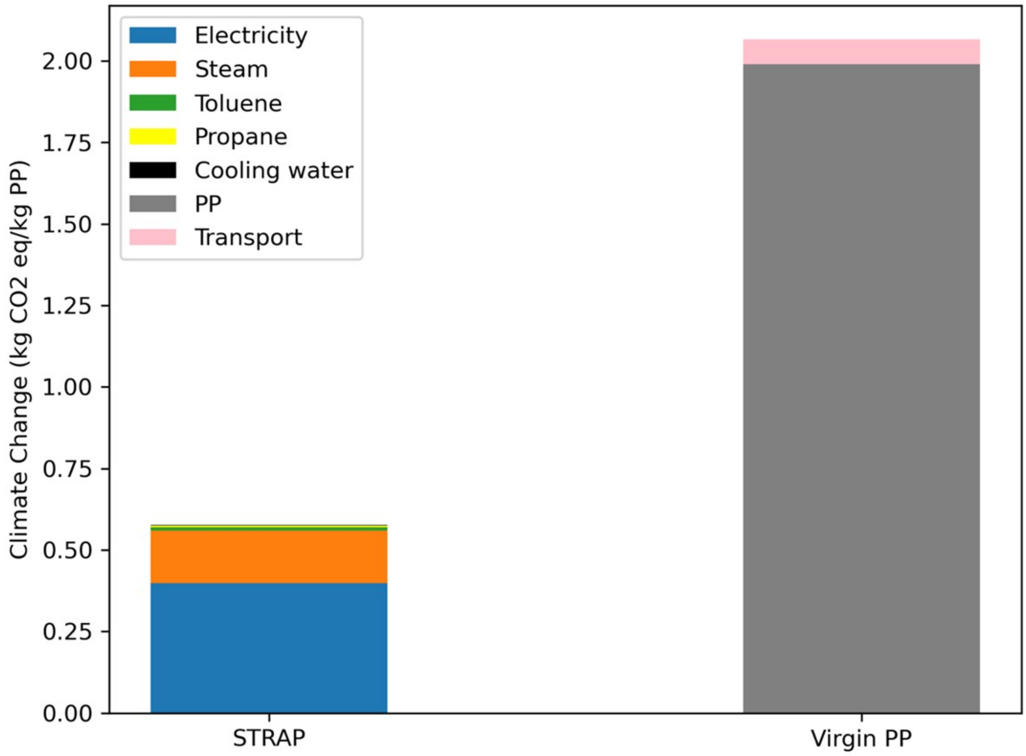

Figure S12. Climate change impact of producing colored PP via the STRAP process in comparison with virgin PP.

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