Supplementary Information

Mapping the end-of-life of chemicals for circular economy opportunities

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This PDF contains: Figures S1-S6, Tables S1-S9, Supplementary References

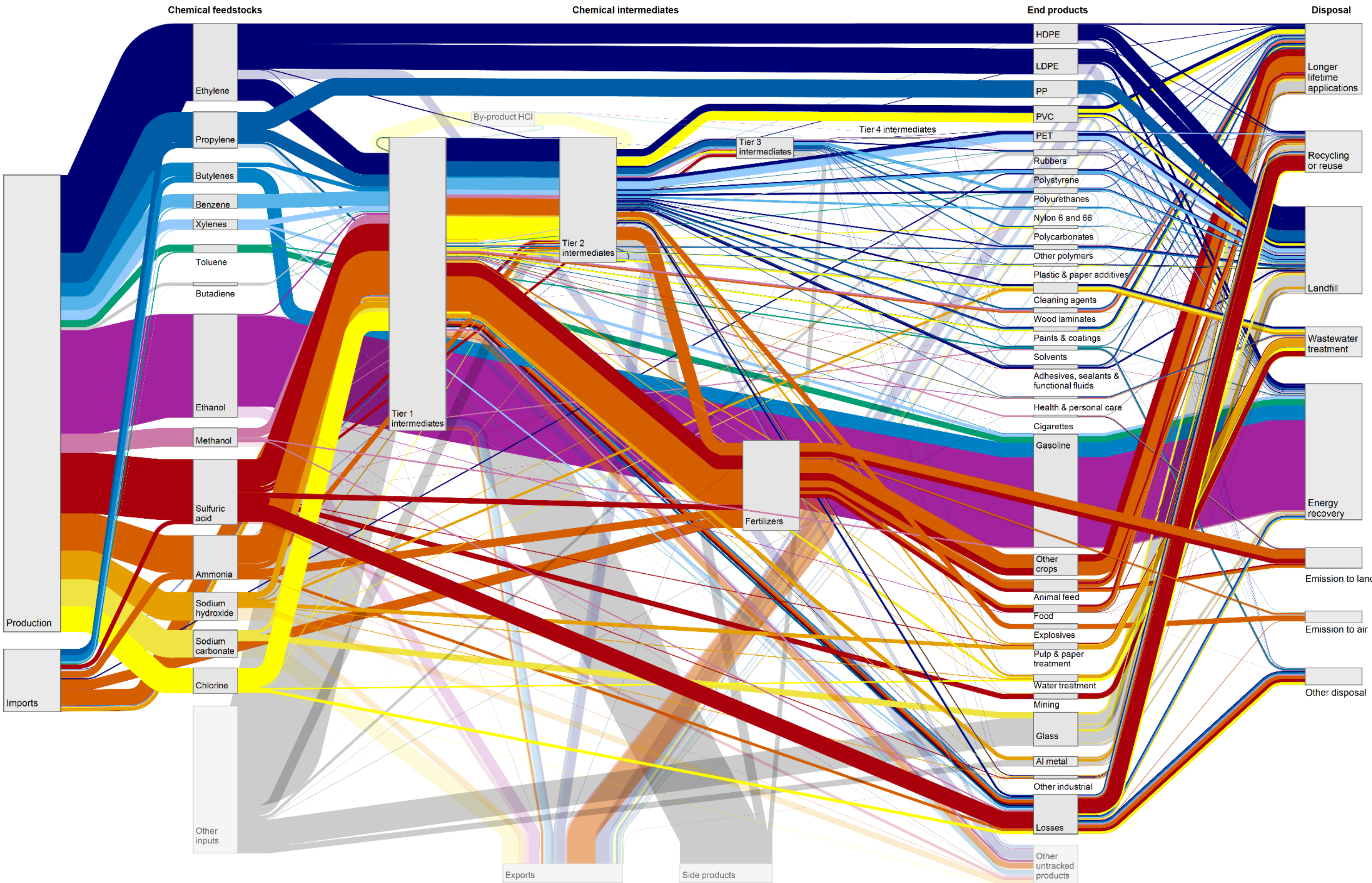

Figure S1. Sankey diagram representing the flow of chemicals in the U.S. in million metric tons from production through to intermediates, final products, and disposal. “Other inputs” include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. “Side products” include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. For visual clarity, emissions to water (0.1 Mt) are combined with wastewater treatment (12.4 Mt). Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

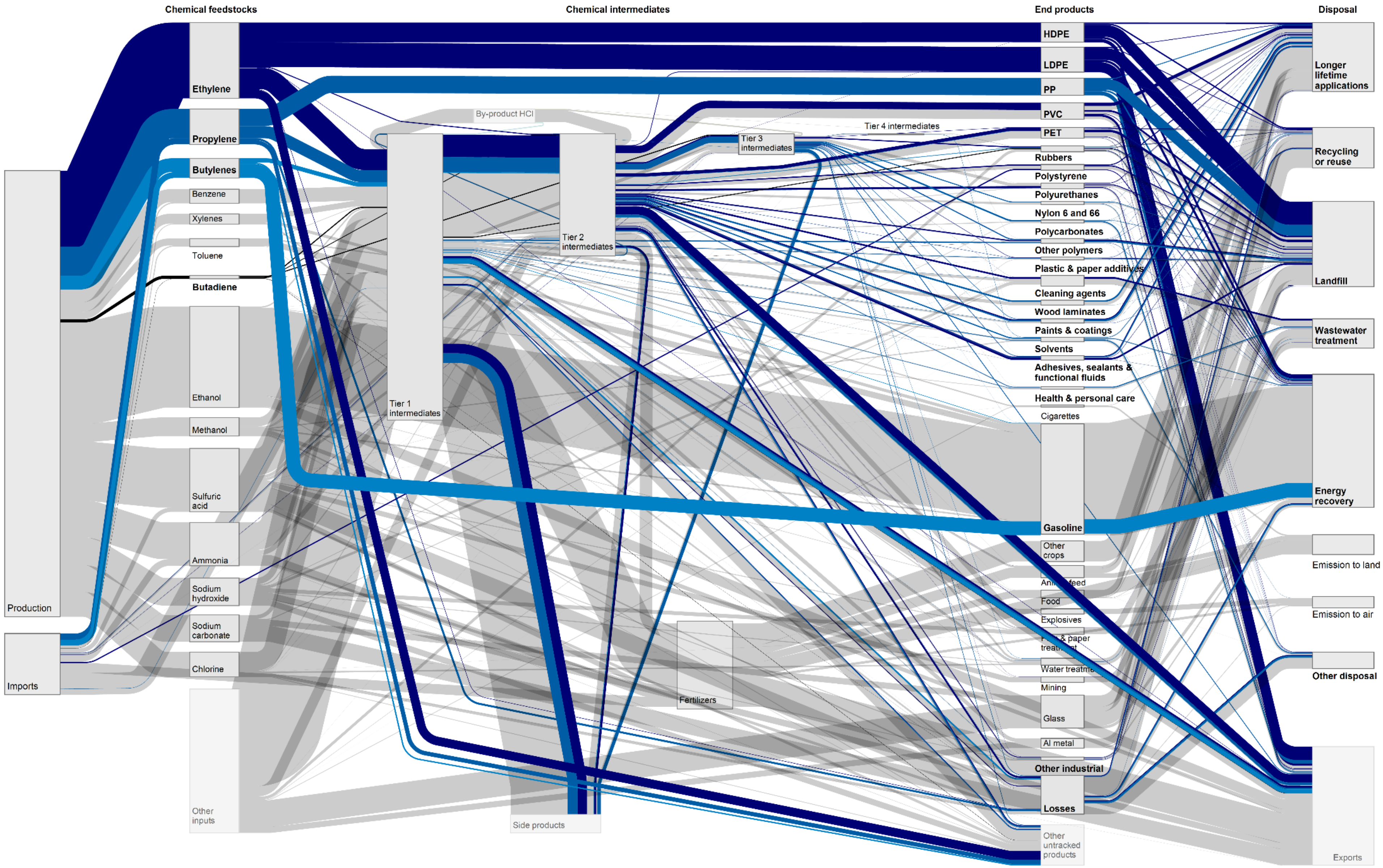

Figure S2. Sankey diagram highlighting the flow of olefins (ethylene, propylene, butylenes, and butadiene) in the U.S. in million metric tons from production through to intermediates, final products, and disposal. Bolded text indicates the relevant end-products and disposal types for olefins. "Other inputs" include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. "Side products" include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

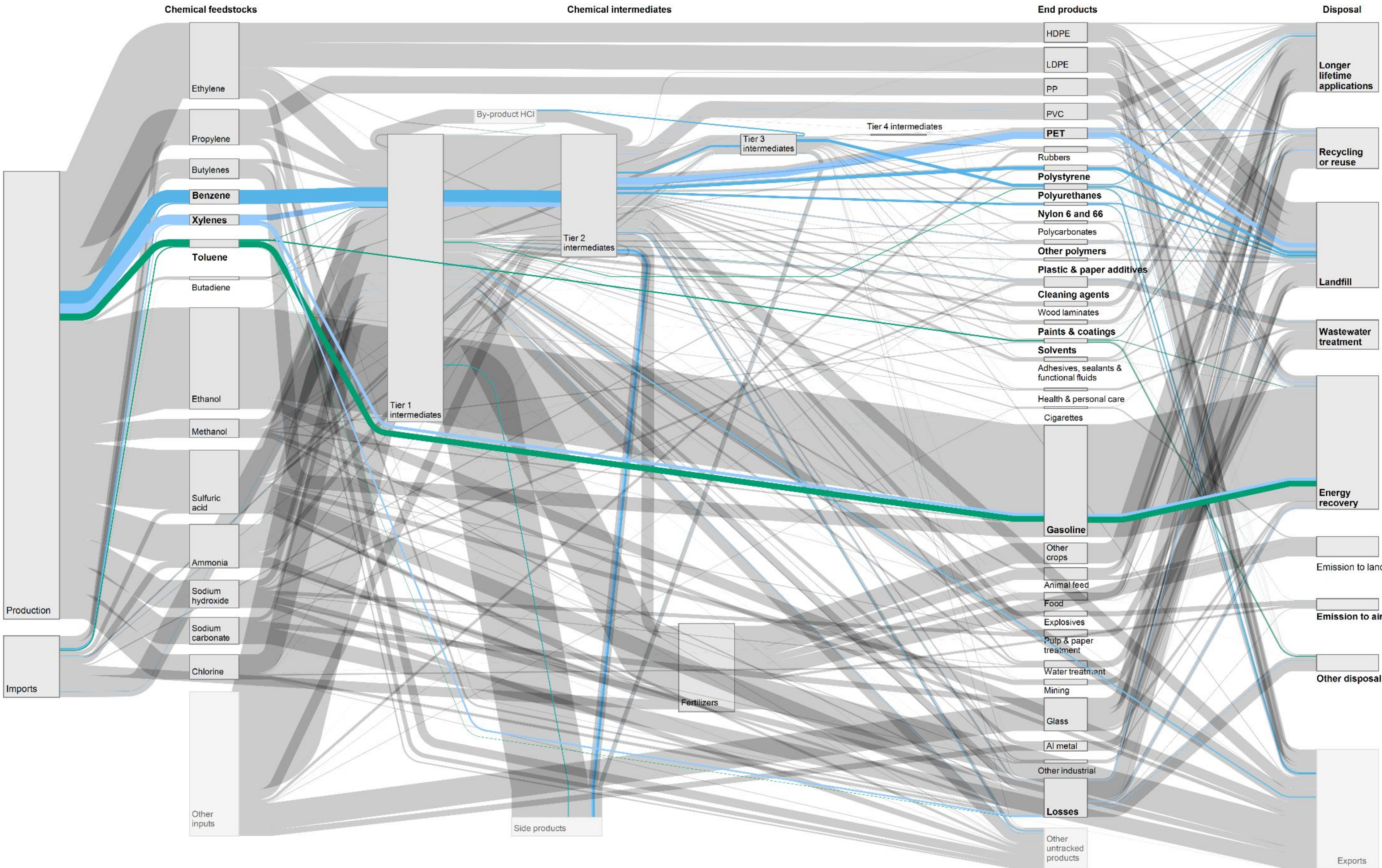

Figure S3. Sankey diagram highlighting the flow of aromatics (benzene, toluene, and xylenes) in the U.S. in million metric tons from production through to intermediates, final products, and disposal. Bolded text indicates the relevant end-products and disposal types for aromatics. "Other inputs" include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. "Side products" include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

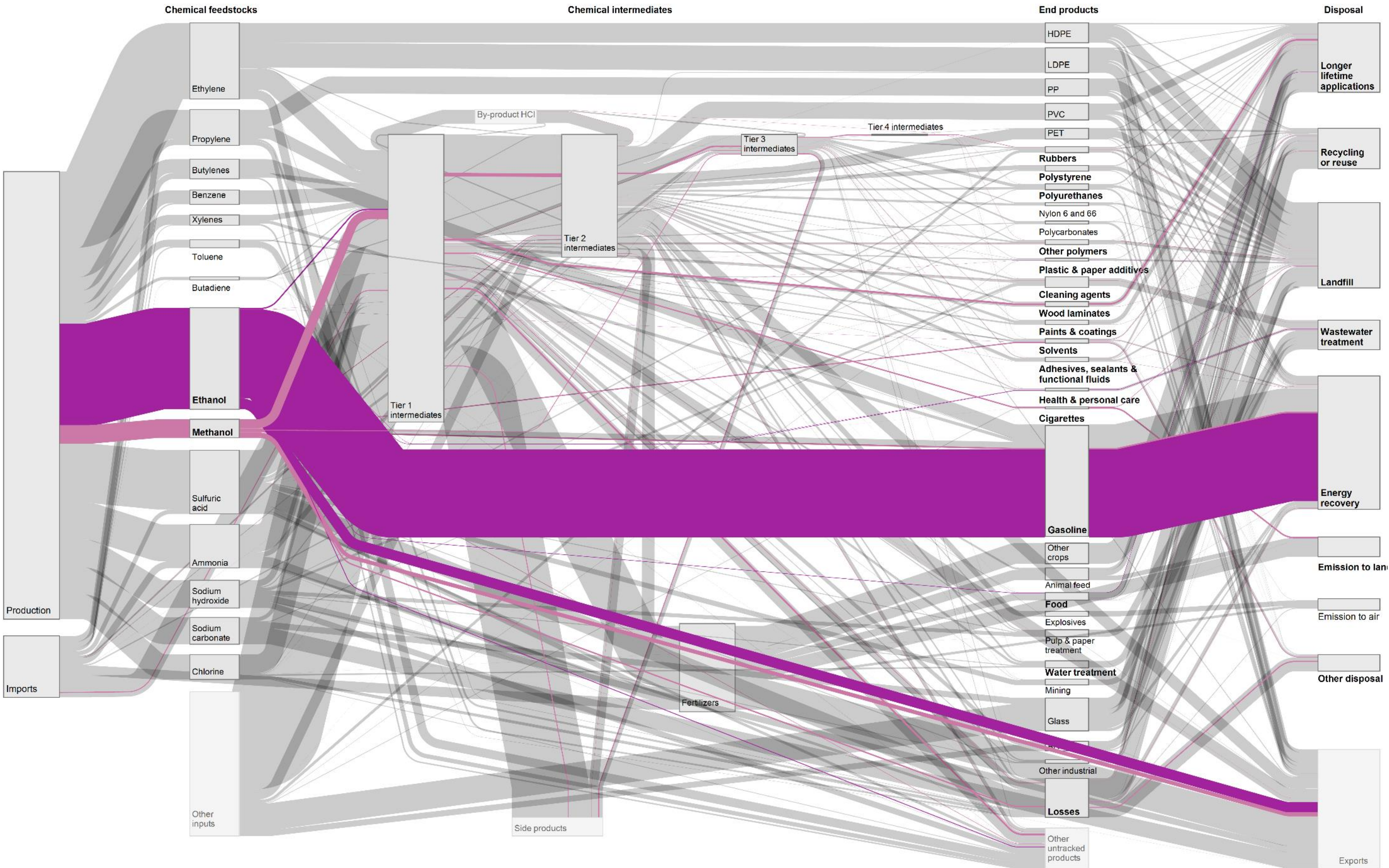

Figure S4. Sankey diagram highlighting the flow of alcohols (ethanol and methanol) in the U.S. in million metric tons from production through to intermediates, final products, and disposal. Bolded text indicates the relevant end-products and disposal types for alcohols. "Other inputs" include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. "Side products" include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

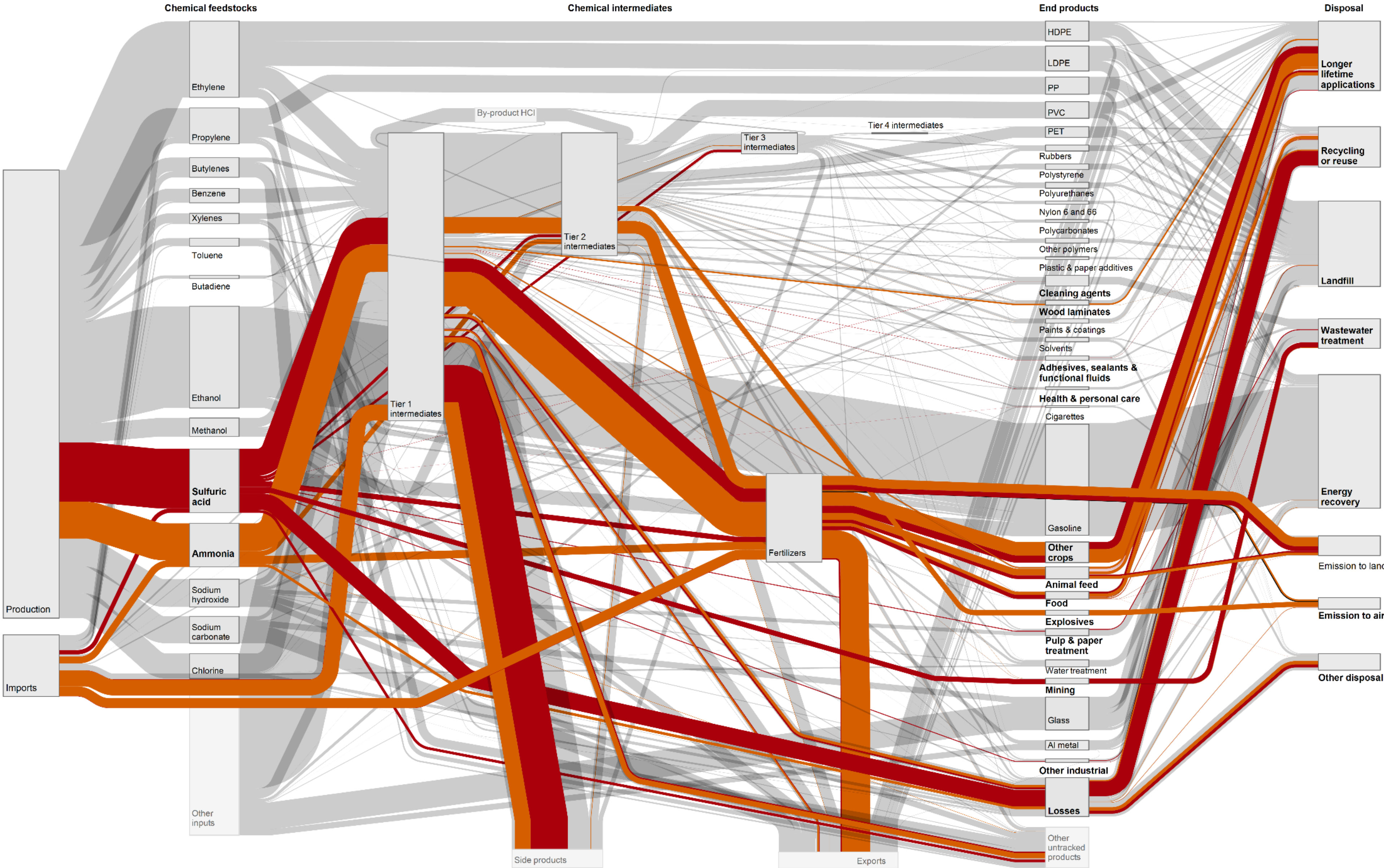

Figure S5. Sankey diagram highlighting the flow of sulfuric acid and ammonia in the U.S. in million metric tons from production through to intermediates, final products, and disposal. Bolded text indicates the relevant end-products and disposal types for sulfuric acid or ammonia. “Other inputs” include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. “Side products” include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

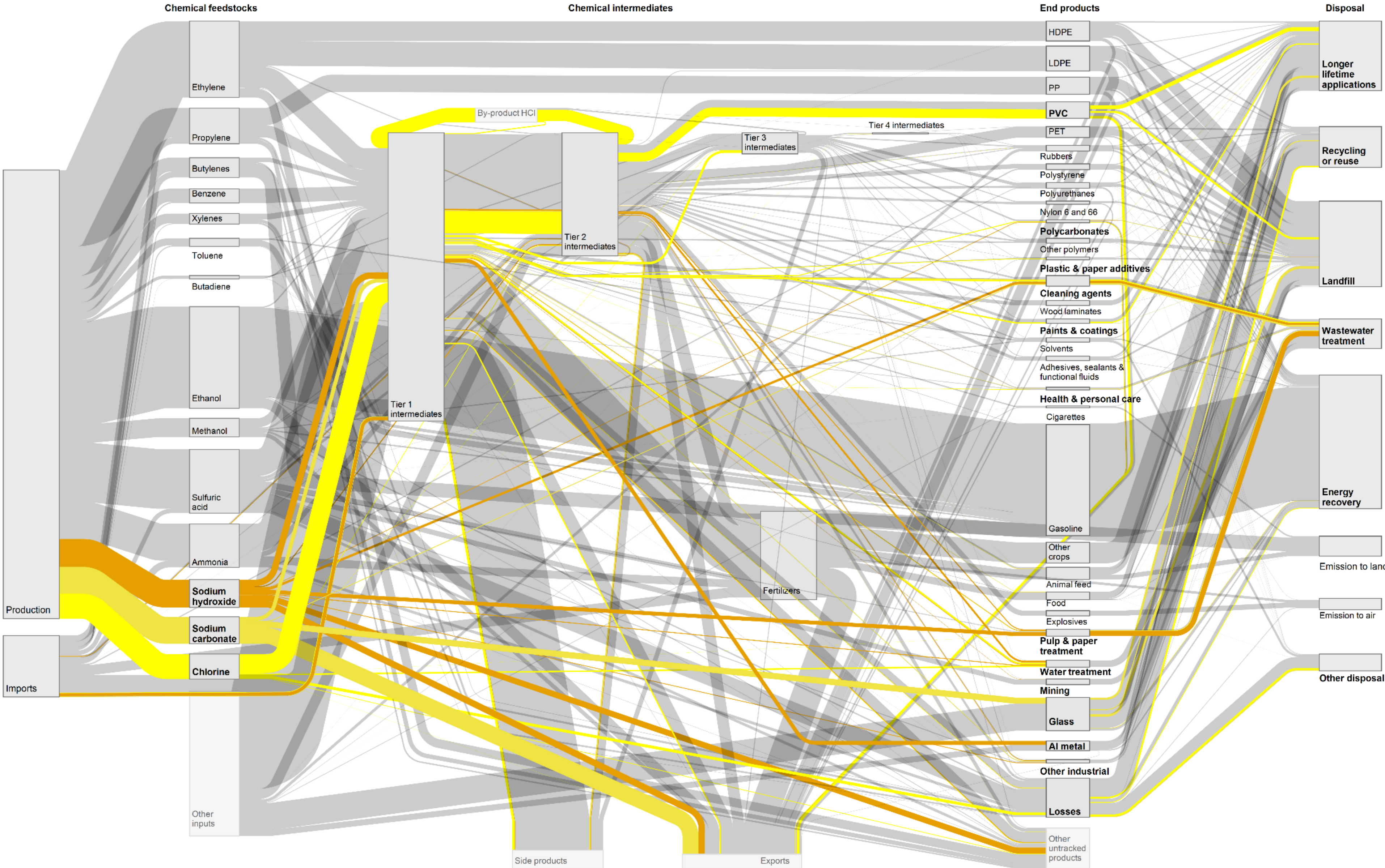

Figure S6. Sankey diagram highlighting the flow of chlor-alkali (sodium hydroxide and chlorine) and sodium carbonate in the U.S. in million metric tons from production through to intermediates, final products, and disposal. Bolded text indicates the relevant end-products and disposal types for chlor-alkali or sodium carbonate. “Other inputs” include feedstocks beyond those listed in the study, such as oxygen, water, hydrogen, or carbon monoxide. “Side products” include by-products that are generated due to chemical reaction stoichiometry, such as carbon dioxide or water. Abbreviations: HCl – hydrochloric acid; HDPE – high density polyethylene; LDPE – low density polyethylene; PP – polypropylene; PVC – polyvinyl chloride; PET – polyethylene terephthalate; Al – aluminum.

Table S1. Overview of the data sources and assumptions used to estimate the production and consumption of chemicals, intermediates, and end-products in this study (continues to page S12). Y = yes; N = no; N/A = not available.

Entry	Production data?	Consumption data?	Ref.	Notes
Ethylene	**Y**	**Y**	**1–3**	
High density polyethylene	Y	Y	1,4–6	
Linear low density polyethylene	Y	Y	1,4,6	
Low density polyethylene	Y	Y	1,4,6	
Ethylene oxide	Y	Y	1,2	
Ethylene dichloride	Y	Y	1,2	
Ethylbenzene	N	N	N/A	Estimated based on ethylene consumption for this end-use and chemical reaction with 100% yield: C_2H_4 + C_6H_6 → C_8H_{10}. Production and consumption were assumed to be equal.
Vinyl acetate	Y	Y	1	
Acetaldehyde	N	Y	1,2	Production and consumption were assumed to be equal.
Ethylene glycol	Y	Y	1,2	
Ethoxylates	Y	Y	1	
Ethanolamines	Y	Y	1	
E-series glycol ethers	Y	Y	1	
Polyethylene glycol	Y	Y	1	
Polyether polyols	Y	Y	1,4	
Vinyl chloride	Y	Y	1,2	
Trichloroethylene	N	N	N/A	Back-calculated based on HFC-125 and HFC-134a requirements using chemical reactions and 100% yield: C_2HCl_3 + 5HF → C_2HF_5 + 3HCl + H_2 and C_2HCl_3 + 4HF → $C_2H_2F_4$ + 3HCl. Production and consumption were assumed to be equal.
Styrene	Y	Y	1,2,7	
Polyvinyl acetate	N	Y	1,4	Production and consumption were assumed to be equal.
Polyvinyl alcohol	N	Y	1	Production and consumption were assumed to be equal.
Ethylene vinyl acetate	N	Y	1,4	Production and consumption were assumed to be equal.
Ethylene vinyl alcohol	N	Y	1	
Polyethylene terephthalate	Y	Y	1,4–6	
Antifreeze	N	N	N/A	Estimated based on ethylene glycol consumption for this end-use. Production and consumption were assumed to be equal.
Polyurethanes	Y	Y	1,4,6,8	
Cleaning agents	N	N	N/A	Estimated based on the consumption of individual chemicals (ethoxylates, acrylic acid, sodium hydroxide, sodium carbonate, ethanolamine, 2-ethylhexanol, polyethylene glycol, E-series glycol ethers, P-series glycol ethers, ethyleneamines, alkylbenzene, methylamine, methyl chloride, silicones, sulfuric acid, sodium silicate, sodium bicarbonate, sodium hypochlorite, calcium hypochlorite) for this end-use. Production and consumption were assumed to be equal.
Herbicides	N	N	N/A	Estimated based on the consumption of individual chemicals (ethanolamine, butylamines, methyl chloride) for this end-use. Production and consumption were assumed to be equal.
Gas treatment	N	N	N/A	Estimated based on the consumption of individual chemicals (ethanolamine, sodium bicarbonate, ethylene glycol, polyethylene glycol, sodium thiosulfate, sodium sulfite) for this end-use. Production and consumption were assumed to be equal.
Cement treatment	N	N	N/A	Estimated based on the consumption of individual chemicals (ethanolamine, ethyleneamines, polycarboxylate ethers) for this end-use. Production and consumption were assumed to be equal.
Metals and mining	N	N	N/A	Estimated based on the consumption of individual chemicals (ethanolamine, 2-ethylhexanol, polyacrylamide, sulfuric acid, acrylic acid, sodium hydrosulfide, sodium sulfide, hydrofluoric acid, nitric acid, sodium cyanide) for this end-use. Production and consumption were assumed to be equal.
Ethyleneamines	Y	Y	1	
Brake fluid & lubricants	N	N	N/A	Estimated based on the consumption of individual chemicals (E-series glycol ethers, polyethylene glycol, 2-ethylhexanol, ethyleneamines, silicones, pentaerythritol, methyl isobutyl ketone) for this end-use. Production and consumption were assumed to be equal.
Health care	N	N	N/A	Estimated based on the consumption of individual chemicals (polyethylene glycol, isopropanol, propylene glycol, methylamine, methylene chloride, acetic anhydride, silicones, methyl cellulose, ethanol,

Entry	Product-ion data?	Consum-ption data?	Ref.	Notes
				sodium bicarbonate) for this end-use. Production and consumption were assumed to be equal.
Personal care	N	N	N/A	Estimated based on the consumption of individual chemicals (polyethylene glycol, isopropanol, propylene glycol, methylamine, methylene chloride, acetic anhydride, silicones, methyl cellulose, ethanol, sodium bicarbonate) for this end-use. Production and consumption were assumed to be equal.
Polycarboxylate ethers	N	N	N/A	
Polyvinyl chloride	Y	Y	1,4,5	
HFC-125	Y	Y	1,9	
HFC-134a	Y	Y	1,9	
Polystyrene	Y	Y	1,4,5	
Acrylonitrile butadiene styrene / styrene-acrylonitrile resin	Y	Y	1,4	
Styrene-butadiene rubber	Y	Y	1,4	
Paints & surface coatings	N	N	N/A	Estimated based on the consumption of individual chemicals (polyvinyl acetate, acrylate esters, isophthalic acid, melamine, ethyleneamines, titanium dioxide, carbon black, E-series glycol ethers, P-series glycol ethers, methyl methacrylate, benzoic acid, phthalic anhydride, methylene chloride, silicones, pentaerythritol, silicas, sodium bicarbonate, epichlorohydrin, n-methyl-2-pyrrolidone, methyl isobutyl ketone, n-butyl acetate) for this end-use. Production and consumption were assumed to be equal.
Adhesives & sealants	N	N	N/A	Estimated based on the consumption of individual chemicals (polyvinyl acetate, polyvinyl alcohol, acrylate esters, polyvinyl butyrate, bisphenol A, methylene chloride, silicones, pentaerythritol, methyl cellulose, melamine, epichlorohydrin) for this end-use. Production and consumption were assumed to be equal.
Paper coatings & additives	N	N	N/A	Estimated based on the consumption of individual chemicals (polyvinyl acetate, acrylate esters, polyacrylamide, titanium dioxide, carbon black, styrene-butadiene latex, silicones, ethanol, polyvinyl alcohol) for this end-use. Production and consumption were assumed to be equal.
Polyvinyl butyral	Y	Y	1	
Plastic additives	N	N	N/A	Estimated based on the consumption of individual chemicals (polyvinyl alcohol, acrylate esters, titanium dioxide, carbon black, 2-ethylhexanol, acrylic acid, benzoic acid, butanol, butylamines) for this end-use. Production and consumption were assumed to be equal.
Propylene	**Y**	**Y**	**1,2,10**	
Polypropylene	Y	Y	1,4,5	
Propylene oxide	Y	Y	1	
Acrylonitrile	Y	Y	1,2	
Cumene	Y	Y	1,11	
Acrylic acid	Y	Y	1,12	
2-ethylhexanol	Y	Y	1,2	
Isopropanol	Y	Y	1,2	
Butanol	Y	Y	1,2	
Epichlorohydrin	Y	Y	1,2	
Propylene glycol	Y	Y	1,13	
Butanediol	Y	Y	1,2	
P-series glycol ethers	Y	Y	1	
Acrylamide	Y	Y	1,14	
Adiponitrile	Y	Y	1	
Nitrile rubber	Y	Y	1	
Carbon fiber	Y	Y	1,15	
Phenol	Y	Y	1,2	
Acetone	Y	Y	1,2	
Acrylate esters	Y	Y	1	
Superabsorbent polymers	Y	Y	1,16	
Solvents	N	N	N/A	Estimated based on the consumption of individual chemicals (2-ethylhexanol, isopropanol, butanol, tetrahydrofuran, ethanol, methanol, acetone, n-methyl-2-pyrrolidone, methyl isobutyl ketone, toluene) for this end-use. Production and consumption were assumed to be equal.
Methyl isobutyl ketone	Y	Y	1,2	
n-butyl acetate	Y	Y	1,17	
Butylamines	Y	Y	1	

Entry	Product-ion data?	Consum-ption data?	Ref.	Notes
Tetrahydrofuran	Y	Y	1,2	
Gamma-butyrolactone	N	N	N/A	Estimated from known butanediol consumption using chemical reaction with 100% yield: $C_4H_{10}O_2 \rightarrow C_4H_6O_2 + 2H_2$ and 100%. Production and consumption were assumed to be equal.
Polybutylene terephthalate	Y	Y	1,4	
Polyacrylamide	Y	Y	1	
Hexamethylene diamine	Y	Y	1,2	
Bisphenol A	Y	Y	1,2,18	
Methyl methacrylate	Y	Y	1	
Pesticides	N	N	N/A	Estimated based on the consumption of individual chemicals (butylamines, methylamine) for this end-use.
N-methyl-2-pyrrolidone	N	N	N/A	Estimated from known gamma-butyrolactone consumption using chemical reaction with 100% yield: $C_4H_6O_2 + CH_5N \rightarrow C_5H_9NO + H_2O$ and 100% yield.
Polycarbonate	Y	Y	1,4,19	
Polymethyl methacrylate	Y	Y	1,4	
Butylenes	**Y**	**Y**	**1,20**	
Gasoline	N	N	N/A	Estimated based on the consumption of individual chemicals (butylenes, toluene, methyl tert butyl ether, ethyleneamines, polyacrylamide, ethanol, xylenes) for this end-use. Production and consumption were assumed to be equal.
Methyl tert-butyl ether	Y	Y	1,2,21	
Ethyl tert-butyl ether	Y	Y	1,22	
Butyl rubber and polyisobutylene	Y	Y	1,4	
Butadiene	**Y**	**Y**	**1,2,20**	
Polybutadiene	Y	Y	1,4	
Benzene	**Y**	**Y**	**1,2,23**	
Nitrobenzene	Y	Y	1,2	
Cyclohexanol / cyclohexanone	N	N	N/A	Estimated from known benzene consumption and chemical reaction: $2C_6H_6 + 5H_2 + O_2 \rightarrow C_6H_{12}O + C_6H_{10}O$. Production and consumption were assumed to be equal.
Alkylbenzene	Y	Y	1	
Aniline	Y	Y	1,2	
Adipic acid	Y	Y	1,2	
Caprolactam	Y	Y	1,2	
Methylene diphenyl diisocyanate	Y	Y	1,2,24	
Nylon 6 / 66	Y	Y	1,4	
Toluene	**Y**	**Y**	**1,2**	
Toluene diisocyanate	Y	Y	1,2,25	
Benzoic acid	Y	Y	1,26	
Sodium / potassium benzoate	N	N	N/A	Estimated from known toluene consumption and chemical reaction with 100% yield: $C_7H_6O_2 + NaOH \rightarrow C_7H_5NaO_2 + H_2O$. Production and consumption were assumed to be equal.
Xylenes	**Y**	**Y**	**1,2**	
Isophthalic acid	Y	Y	1,2	
Terephthalic acid	Y	Y	1,2	
Dimethyl terephthalate	Y	Y	1	
Phthalic anhydride	Y	Y	1,2	
Methanol	**Y**	**Y**	**1,2,27**	
Formaldehyde	Y	Y	1,2,28	
Acetic acid	Y	Y	1,2	
Biodiesel	N	N	N/A	Estimated based on the consumption of methanol for this end-use. Production and consumption were assumed to be equal.
Methylamines	N	N	N/A	Estimated based on the consumption of methanol for this end-use. Production and consumption were assumed to be equal.
Methyl chloride	Y	Y	1,2,20	
Polyacetal resins	Y	Y	1,4	
Pentaerythritol	Y	Y	1,20	
Acetic anhydride	Y	Y	1,2	
Methylene chloride	Y	Y	1,29	
Methyl chlorosilanes	N	N	N/A	Estimated based on the consumption of methyl chloride for this end-use. Production and consumption were assumed to be equal.
Methyl cellulose	Y	Y	1	
Cellulose acetates	Y	Y	1,30	

Entry	Product-ion data?	Consum-ption data?	Ref.	Notes
Cigarettes	N	N	N/A	Estimated assuming that 100% of cellulose acetates are consumed for this end-use. Production and consumption were assumed to be equal.
Chloroform	Y	Y	1,2	
HFC-32	Y	Y	1,9	
Silicones	Y	Y	1	
Carbon tetrachloride	Y	Y	1,31	
HCFC-22	Y	Y	1	
Refrigerants and air conditioning	N	N	N/A	Estimated based on the consumption of individual chemicals (HFC-32, HCFC-22, HFC-125, HFC-134a, carbon tetrachloride, and hydrofluoric acid) for this end-use. Production and consumption were assumed to be equal.
Fluoropolymers	N	N	N/A	Estimated based on the consumption of HCFC-22 for this end-use. Production and consumption were assumed to be equal.
Silicone rubbers and elastomers	N	N	N/A	Estimated based on the consumption of silicones for this end-use. Production and consumption were assumed to be equal.
Ethanol	**Y**	**Y**	**1,32**	
Food	N	N	33	Estimated based on the consumption of individual chemicals (ethanol, silicas, sodium bicarbonate, fertilizers, sodium/potassium benzoate) for this end-use; food mass itself is not included. 19% of total fertilizer was assumed to be used for food based on the distribution of U.S. crop growth by end-use (data in ref. at left). Production and consumption were assumed to be equal.
Ammonia	**Y**	**Y**	**1,34,35**	
Ammonia fertilizer	Y	Y	1,35	
Urea	Y	Y	1,35	
Nitric acid	Y	Y	1,35	
Ammonium phosphate fertilizers	Y	Y	1,35	
Complex NPK fertilizers	Y	Y	1,35	
Ammonium sulfate fertilizers	Y	Y	1,35	
Hydrogen cyanide	Y	Y	1,36	
Urea-based fertilizers	Y	Y	35	
Fertilizers	N	N	N/A	Estimated based on the consumption of individual chemicals (ammonia fertilizers, ammonium phosphate fertilizers, complex NPK fertilizers, ammonium sulfate fertilizers, ammonium nitrate fertilizers, urea based fertilizers) for this end-use; losses from plant growth (70% nitrogen use efficiency) are accounted for. Production and consumption were assumed to be equal.
Animal feeds	N	N	33	Estimated based on the consumption of individual chemicals (urea, phosphoric acid, sodium bicarbonate, methylamine, acetaldehyde, silicas, fertilizers) for this end-use; biomass weight itself is not included. 26% of total fertilizer was assumed to be used for animal feed production based on the distribution of U.S. crop growth by end-use (data in ref. at left). Production and consumption were assumed to be equal.
Other crops	N	N	33	Estimated based on the consumption of fertilizers for this end-use; crop mass itself is not included. 55% of total fertilizer was assumed to be used for other crops based on the distribution of U.S. crop growth by end-use (data in ref. at left). Production and consumption were assumed to be equal.
Melamine	Y	Y	1	
Ammonium nitrate	Y	Y	1,35,37	
Sodium cyanide	Y	Y	1	
Wood laminates	N	N	N/A	Estimated based on the consumption of individual chemicals (melamine, formaldehyde, urea, butanol, phenol, ethanolamine) for this end-use; wood mass itself is not included. Production and consumption were assumed to be equal.
Ammonium nitrate fertilizers	Y	Y	1,35,37	
Ammonium nitrate explosives	Y	Y	1	
Chlorine	**Y**	**Y**	**1,38**	
Phosgene	Y	Y	1,2,39	
Aluminum chloride	Y	Y	1	
Sodium hypochlorite	Y	Y	1,40	
Calcium hypochlorite	Y	Y	1,41	
Titanium dioxide	Y	Y	1,42	
Pulp and paper treatment	N	N	N/A	Estimated based on the consumption of individual chemicals (chlorine, sodium hydroxide, polyvinyl acetate, methylamine, aluminum chloride,

Entry	Production data?	Consumption data?	Ref.	Notes
				sulfuric acid, aluminum sulfate, sodium aluminate, sodium hydrosulfide, sodium hydrosulfite, sodium sulfide, sodium sulfite, sodium silicate, silicas) for this end-use. Production and consumption were assumed to be equal.
Water treatment	N	N	N/A	Estimated based on the consumption of individual chemicals (chlorine, sodium hydroxide, acrylic acid, polyacrylamide, methylamine, aluminum chloride, sodium hypochlorite, aluminum sulfate, sodium aluminate, sodium sulfite, sodium thiosulfate, sodium bicarbonate) for this end-use. Production and consumption were assumed to be equal.
Catalysts	N	N	N/A	Estimated based on the consumption of individual chemicals (aluminum chloride, sodium aluminate, sodium silicate, silicas) for end-use. Production and consumption were assumed to be equal.
Sodium hydroxide	**Y**	**Y**	**1,43,44**	
Aluminum oxide	Y	Y	45	
Sodium hydrosulfide	Y	Y	1	
Sodium hydrosulfite	Y	Y	1	
Sodium sulfide	Y	Y	1	
Sodium sulfite	Y	Y	1	
Sodium thiosulfate	Y	Y	1	
Textiles processing	N	N	N/A	Estimated based on the consumption of individual chemicals (sodium hydroxide, sodium hydrosulfite) for this end-use. Production and consumption were assumed to be equal.
Aluminum metal	Y	Y	46	
Aluminum sulfate	Y	Y	1,47	
Sodium aluminate	Y	Y	1	
Sulfuric acid	**Y**	**Y**	**1,48,49**	
Phosphoric acid	Y	Y	1,50	
Hydrofluoric acid	Y	Y	1	
Lead acid batteries	N	N	N/A	Estimated based on the consumption of individual chemicals (sulfuric acid, silicas) for this end-use; other non-chemical components were not included. Production and consumption were assumed to be equal.
Sodium carbonate	**Y**	**Y**	**1,51,52**	
Glass, flat	Y	Y	53–55	
Glass, container	Y	Y	53–55	
Glass, other	Y	Y	53–55	
Sodium silicate	Y	Y	1,56	
Sodium bicarbonate	Y	Y	1	
Silicas	Y	Y	1,57	
Adsorbents	N	N	N/A	Estimated based on the consumption of individual chemicals (sodium silicate, silicas) for this end-use. Production and consumption were assumed to be equal.

Table S2. End-of-life assumptions for the end-products included in this study (continues to page S15). N/A = not available.

End-product	Dispose (%)	Longer life (%)	Land -fill (%)	Recycle or reuse (%)	Energy recover (%)	Incin-erate (%)	Emit to air (%)	Emit to land (%)	Emit to water (%)	Waste-water (%)	Other (%)	Notes	Ref.
ABS & other resins	87	13	70	22	8	0	0	0	0	0	0	Data from 2019.	6
Adhesives & sealants	6	94	100	0	0	0	0	0	0	0	0	Assume products go to electronics (5-year lifetime), construction (50-year), and consumer products (1-year), for average of 17 years. All disposed is landfilled.	N/A
Adsorbents	100	0	100	0	0	0	0	0	0	0	0	Assume all are landfilled.	N/A
Aluminum metal	86.5	13.5	68	17	14	0	0	0	0	0	1	Data from 2018.	58
Animal feed	75	25	0	50	0	0	0	50	0	0	0	Using nitrogen use efficiency of livestock, assume 75% of incoming feed is released as manure. Half is reused as fertilizer while the other half is disposed.	59
Antifreeze	100	0	88	12	0	0	0	0	0	0	0	Data from 1999.	60
Biodiesel	100	0	0	0	100	0	0	0	0	0	0	Assume biodiesel is burned for energy.	N/A
Brake fluid & lubricants	100	0	0	40	46	0	0	0	14	0	0	Data from 2006.	61
Carbon fiber	30	70	98	0	0	2	0	0	0	0	0	30% loss during manufacturing. Assume 50-year lifetime in durable goods.	62,63
Catalysts	50	50	70	30	0	0	0	0	0	0	0	Assume 2-year lifetime. Data from 1996.	64
Cement & concrete	100	0	0	0	0	0	0	0	0	100	0	Assume all chemicals used for grinding end up in wastewater treatment.	N/A
Cigarettes	100	0	25	0	0	0	0	75	0	0	0	Data from 2009.	65
Cleaning agents	100	0	0	0	0	0	0	0	2.4	97.6	0	Assume all end up in water. 84% sent to wastewater treatment and 16% to septic tanks (U.S. average); ~15% of septic tanks fail, so 2.4% go to groundwater.	66,67
Explosives	100	0	0	0	0	0	100	0	0	0	0	Assume all explosives are detonated and released to the environment.	N/A
Fertilizer, ammonia	30	70	0	0	0	0	29	71	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization rates reported in second ref. at right, with remainder assumed to be emitted to land.	68,69
Fertilizer, ammonium nitrate	30	70	0	0	0	0	3	97	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization rates reported in second ref. at right, with remainder assumed to be emitted to land.	68,69
Fertilizer, ammonium phosphate	30	70	0	0	0	0	3	97	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization rates reported in second ref. at right, with remainder assumed to be emitted to land.	68,69
Fertilizer, ammonium sulfate	30	70	0	0	0	0	2	98	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization	68,69

End-product	Dispose (%)	Longer life (%)	Land -fill (%)	Recycle or reuse (%)	Energy recover (%)	Incin-erate (%)	Emit to air (%)	Emit to land (%)	Emit to water (%)	Waste-water (%)	Other (%)	Notes	Ref.
												rates reported in second ref. at right, with remainder assumed to be emitted to land.	
Fertilizer, complex NPK	30	70	0	0	0	0	3	97	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization rates reported in second ref. at right, with remainder assumed to be emitted to land.	68,69
Fertilizer, urea	30	70	0	0	0	0	32	68	0	0	0	Longer lifetime is based on the nitrogen use efficiency of the U.S. (first ref. at right). Air emissions are based on volatization rates reported in second ref. at right, with remainder assumed to be emitted to land.	68,69
Food	31	69	37	42	9	0	0	5	0	4	3	Data from 2019 includes residential, manufacturing, retailers, and distributors. Recycling includes compost, donation, animal feed, and anaerobic digestion.	70
Gas treatment	100	0	0	0	0	0	0	0	0	100	0	Assume all consumed amines sent to wastewater treatment.	N/A
Gasoline	100	0	0	0	100	0	0	0	0	0	0	Assume all gasoline is burned for energy.	N/A
Glass, container	100	0	55	31	13	0	0	0	0	0	0	Data from 2018.	N/A
Glass, flat	51	49	86	0	13	0	0	0	0	0	0	Data from 2018 for “durable” glass.	58
Glass, other	3	97	100	0	0	0	0	0	0	0	0	Assumed to be fiberglass for insulation (50-year lifetime) and automotives (10-year) for average of 30 years.	N/A
HDPE	92	8	78	9	13	0	0	0	0	0	1	Average from refs. (2015, 2018-2019).	5,6,58,71
Health care	100	0	3	0	0	0	0	0	2.3	94.7	0	3% of production thrown away; assume remainder sent to wastewater and septic tanks (see cleaning agents).	72
Herbicides	100	0	0	0	0	0	0	0	100	0	0	Herbicides kill aqueous weeds, so assume all ends up in water.	N/A
LDPE	96	4	79	4	14.5	0	0	0	0	0	1	Average from refs. (2015, 2018-2019).	5,6,58,71
LLDPE	96	4	79	5	14.5	0	0	0	0	0	1	Average from refs. (2015, 2018-2019).	5,6,58,71
Lead acid batteries	20	80	0	0	0	0	0	0	0	100	0	Assume 5-year lifetime and that batteries are recycled, during which sulfuric acid is neutralized and sent to wastewater.	58
Losses, ammonia	100	0	3	21	12	13	0	0	0	0	51	Data from 2021.	73
Losses, benzene	100	0	0	47	16	1	2	0	0	0	34	Data from 2021.	73
Losses, butanol	100	0	1	19	30	3	7	0	0	0	40	Data from 2021.	73
Losses, ethylene	100	0	0	12	35	1	0	0	0	0	52	Data from 2021.	73
Losses, ethylene dichloride	100	0	0	67	0	0	0	0	0	0	33	Data from 2021.	73
Losses, ethylene glycol	100	0	5	64	4	1	0.5	0	0	3	22.5	Data from 2021.	73
Losses, ethylene oxide	100	0	0	0	2	1.5	0	0	0	0	96.5	Data from 2021.	73
Losses, formaldehyde	100	0	11	17	18	4	0	0	0	3	47	Data from 2021.	73
Losses, methanol	100	0	1	23	20	2	5	0	0	1	48	Data from 2021.	73
Losses, phenol	100	0	2.5	56	14	1	3	0	0	1	22.5	Data from 2021.	73
Losses, propylene	100	0	0	9	44	1	0	0	0	0	46	Data from 2021.	73

End-product	Dispose (%)	Longer life (%)	Land -fill (%)	Recycle or reuse (%)	Energy recover (%)	Incin-erate (%)	Emit to air (%)	Emit to land (%)	Emit to water (%)	Waste-water (%)	Other (%)	Notes	Ref.
Losses, propylene oxide	100	0	0	0	61	0	1	0	0	0	38	Data from 2021.	73
Losses, sulfuric acid	100	0	0	90	0	0	0.5	0	0	0	9.5	Data from 2021.	73
Losses, styrene	100	0	3	3	35	4	39	0	0	0	16	Data from 2021.	73
Losses, toluene	100	0	0	70	13	2	1	0	0	0	14	Data from 2021.	73
Losses, xylenes	100	0	0	42	36	3	3	0	0	0	16	Data from 2021.	73
Metals & mining	100	0	0	0	0	0	0	0	0	100	0	Assume all mining chemicals end up in wastewater treatment.	74
Nylon 6 & 66	89	11	92	0	8	0	0	0	0	0	0	Data from 2019.	6
Other crops	0.1	99.9	100	0	0	0	0	0	0	0	0	Assume most crops have long lifetimes.	
Other polymers	94	6	82	7	9	0	0	0	0	0	3	Average from refs. for “other” (data from 2015, 2018-2019).	5,6,58,71
Paints & surface coatings	10	90	73	27	0	0	0	0	0	0	0	Data from 2007.	75,76
Paper coatings & additives	100	0	41	53	6	0	0	0	0	0	0	Average from refs. for paper and paperboard (2018-2019).	58,77
PC	79	21	82	9.5	8.5	0	0	0	0	0	0	Data from 2019.	6
Personal care	100	0	6	0	0	0	0	0	2.2	91.8	0	6% of production thrown away; assume remainder sent to wastewater and septic tanks (see cleaning agents).	72
Pesticides	18	88	0	0	0	0	0	96	0.4	0	3.6	Data from 2015.	78
PET	92	8	71	16	13	0	0	0	0	0	0	Average from refs. (2015, 2018-2019).	5,6,58,71
Plastic additives	100	0	80	6	13	0	0	0	0	0	1	Average from refs. for total of all plastic types (data from 2015, 2018-2019).	5,6,58,71
PP	94	6	86	1	12	0	0	0	0	0	1	Average from refs. (2015, 2018-2019).	5,6,58,71
PS	84	16	83	2	15	0	0	0	0	0	0	Average from refs. (2015, 2018-2019).	5,6,58,71
Pulp & paper treatment	100	0	0	0	0	0	0	0	0	100	0	Assume all is sent to wastewater.	N/A
PUR	71	29	78.5	9	8.5	0	0	0	0	0	0	Average from refs. (2016 and 2019).	6,8
PVC	39	61	85	1	13	0	0	0	0	0	1	Average from refs. (2015, 2018-2019).	5,6,58,71
Refrigerants & air conditioning	8	92	79	21	0	0	0	0	0	0	0	A/C units have 12.5-year lifetime. Assume recycled or landfilled according to ref. (2021).	79
Rubbers	87	13	45	24	31	0	0	0	0	0	0	Average from refs. (2018-2019).	6,58
Solvent	100	0	0.4	39	19	2.3	4.2	0	0	0.3	35	Data for butanol, methanol, n-methylpyrrolidone, and methyl isobutyl ketone, as well as an estimated average for non-TRI chemicals (2021).	73
Superabsorbent polymers	100	0	80	0	20	0	0	0	0	0	0	Data for diapers only (2018).	80
Textiles processing	100	0	0	0	0	0	0	0	0	100	0	Assume all is sent to wastewater.	N/A
Water treatment	100	0	36	0	0	0	0	0	0	64	0	Assume the polymers and aluminas are used as coagulants and landfilled. Other components in wastewater.	N/A
Wood laminates	5	95	100	0	0	0	0	0	0	0	0	Assume 20-year lifetime, then landfill.	N/A

Table S3. Chemical reactions for the chemical intermediates included in this study (continues to page S17).

Target chemical	Target category	Starting chemical	Chemical reaction
Polyethylene	End-product	Ethylene	$C_2H_4 \rightarrow (C_2H_4)_n$
Ethylene oxide [a]	Tier 1 intermediate	Ethylene	$2C_2H_4 + O_2 \rightarrow 2C_2H_4O$
Ethylene dichloride	Tier 1 intermediate	Ethylene	$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$
Ethylbenzene	Tier 1 intermediate	Ethylene	$C_2H_4 + C_6H_6 \rightarrow C_8H_{10}$
Vinyl acetate	Tier 1 intermediate	Ethylene	$2C_2H_4 + 2C_2H_4O_2 + O_2 \rightarrow 2C_4H_6O_2 + 2H_2O$
Acetaldehyde	Tier 1 intermediate	Ethylene	$C_2H_4 + H_2O \rightarrow C_2H_4O$
Ethylene glycol	Tier 2 intermediate	Ethylene oxide	$C_2H_4O + H_2O \rightarrow C_2H_6O_2$
Ethanolamines	Tier 2 intermediate	Ethylene oxide	$C_2H_4O + NH_3 \rightarrow C_2H_7NO$
E-series glycol ethers	Tier 2 intermediate	Ethylene oxide	$C_2H_4O + C_4H_{10}O \rightarrow C_6H_{14}O_2$
Polyethylene glycol	Tier 2 intermediate	Ethylene oxide	$C_2H_4O + C_2H_6O_2 \rightarrow (C_2H_4O)_n + 2H_2O$
Vinyl chloride	Tier 2 intermediate	Ethylene dichloride	$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$
Trichloroethylene	Tier 2 intermediate	Ethylene dichloride	$C_2H_4Cl_2 + 2Cl_2 \rightarrow C_2HCl_3 + 3HCl$
Styrene	Tier 2 intermediate	Ethylbenzene	$C_8H_{10} \rightarrow C_8H_8 + H_2$
Polyvinyl acetate	Tier 2 intermediate	Vinyl acetate	$C_4H_6O_2 \rightarrow (C_4H_6O_2)_n$
Polyvinyl alcohol	Tier 2 intermediate	Vinyl acetate	$C_4H_6O_2 + 2CH_4O \rightarrow 3C_2H_4O + H_2O$
Ethylene vinyl acetate [b]	Tier 2 intermediate	Vinyl acetate	$C_4H_6O_2 + 18C_2H_4 \rightarrow (C_2H_4)_{18}(C_4H_6O_2)$
Ethylene vinyl alcohol [c]	Tier 2 intermediate	Vinyl acetate	$C_4H_6O_2 + C_2H_4 \rightarrow (C_2H_4O\text{-}C_2H_4)_n$
Polyethylene terephthalate	End-product	Ethylene glycol	$C_2H_6O_2 + C_8H_6O_4 \rightarrow C_{10}H_8O_4 + 2H_2O$
Polyurethanes	End-product	Ethylene glycol	$C_{15}H_{10}N_2O_2 + C_9H_6N_2O_2 + C_2H_6O_2 + CH_{10}O_2 + 2H_2O \rightarrow (C_{27}H_{36}N_2O_{10})_n + N_2$
Ethyleneamines	Tier 3 intermediate	Ethanolamines	$C_2H_7NO + NH_3 \rightarrow C_2H_8N_2 + H_2O$
Polyvinyl chloride	End-product	Vinyl chloride	$C_2H_3Cl \rightarrow (C_2H_3Cl)_n$
HFC-125	Tier 3 intermediate	Trichloroethylene	$C_2HCl_3 + 5HF \rightarrow C_2HF_5 + 3HCl + H_2$
HFC-134a	Tier 3 intermediate	Trichloroethylene	$C_2HCl_3 + 4HF \rightarrow C_2H_2F_4 + 3HCl$
Polystyrene	Tier 3 intermediate	Styrene	$C_8H_8 \rightarrow (C_8H_8)_n$
Acrylonitrile butadiene styrene	End-product	Styrene	$C_8H_8 + C_3H_3N + C_4H_6 \rightarrow (C_{15}H_{17}N)_n$
Styrene-butadiene rubber	End-product	Styrene	$C_8H_8 + C_4H_6 \rightarrow (C_{12}H_{14})_n$
Polyvinyl butyral	End-product	Polyvinyl alcohol	$2C_2H_4O + C_4H_8O \rightarrow (C_8H_{14}O_2)_n + H_2O$
Polypropylene	End-product	Propylene	$C_3H_6 \rightarrow (C_3H_6)_n$
Propylene oxide	Tier 1 intermediate	Popylene	$C_3H_6 + NaOH + HOCl \rightarrow C_3H_6O + NaCl + H_2O$
Acrylonitrile	Tier 1 intermediate	Propylene	$C_3H_6 + NH_3 + 1.5O_2 \rightarrow C_3H_3N + 3H_2O$
Cumene	Tier 1 intermediate	Propylene	$C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$
Acrylic acid	Tier 1 intermediate	Propylene	$2C_3H_6 + 3O_2 \rightarrow 2C_3H_4O_2 + 2H_2O$
2-ethylhexanol	Tier 1 intermediate	Propylene	$2C_3H_6 + 3CO + 6H_2 \rightarrow C_8H_{18}O + CO_2$
Isopropanol	Tier 1 intermediate	Propylene	$C_3H_6 + H_2O \rightarrow C_8H_8O$
Butanol	Tier 1 intermediate	Propylene	$C_3H_6 + CO + 2H_2 \rightarrow C_4H_{10}O$
Epichlorohydrin	Tier 1 intermediate	Propylene	$C_3H_6 + 2Cl_2 + NaOH \rightarrow C_3H_5ClO + NaCl + 2HCl$
Propylene glycol	Tier 2 intermediate	Propylene oxide	$C_3H_6O + H_2O \rightarrow C_3H_8O_2$
Butanediol	Tier 2 intermediate	Propylene oxide	$C_2H_2 + 2CH_2O + 2H_2 \rightarrow C_4H_{10}O_2$
P-series glycol ethers	Tier 2 intermediate	Propylene oxide	$C_3H_6O + CH_4O \rightarrow C_4H_{10}O_2$
Acrylamide	Tier 2 intermediate	Acrylonitrile	$C_3H_3N + H_2O \rightarrow C_3H_5NO$
Adiponitrile	Tier 2 intermediate	Acrylonitrile	$2C_3H_3N \rightarrow C_6H_8N_2$
Nitrile rubber [d]	Tier 2 intermediate	Acrylonitrile	$C_3H_3N + C_4H_6 \rightarrow (C_3H_3N)(C_4H_6)$
Carbon fiber	Tier 2 intermediate	Acrylonitrile	$C_3H_3N + O_2 \rightarrow 2C + CO_2 + NH_3$
Phenol	Tier 2 intermediate	Cumene	$C_9H_{12} + O_2 \rightarrow C_6H_6O + C_3H_6O$
Acetone	Tier 2 intermediate	Cumene	$C_9H_{12} + O_2 \rightarrow C_6H_6O + C_3H_6O$
Acrylate esters	Tier 2 intermediate	Acrylic acid	$C_3H_4O_2 + C_4H_{10}O \rightarrow C_7H_{12}O_2 + H_2O$
Superabsorbent polymers	End-product	Acrylic acid	$C_3H_4O_2 \rightarrow (C_3H_4O_2)_n$
Methyl isobutyl ketone	Tier 2 intermediate	Isopropanol	$2C_3H_6O \rightarrow C_6H_{12}O$
n-butyl acetate	Tier 2 intermediate	Butanol	$C_4H_{10}O + C_2H_4O_2 \rightarrow C_6H_{12}O_2 + H_2O$
Butylamines	Tier 2 intermediate	Butanol	$C_4H_{10}O + NH_3 \rightarrow C_4H_{11}N + H_2O$
Tetrahydrofuran	Tier 3 intermediate	Butanediol	$C_4H_{10}O_2 \rightarrow C_4H_8O + H_2O$
Gamma-butyrolactone	Tier 3 intermediate	Butanediol	$C_4H_{10}O_2 \rightarrow C_4H_6O_2 + 2H_2$
Polybutylene terephthalate	End-product	Butanediol	$C_4H_{10}O_2 + C_8H_6O_4 \rightarrow (C_{12}H_{12}O_4)_n$
Polyacrylamide	Tier 3 intermediate	Acrylamide	$C_3H_5NO \rightarrow (C_3H_5NO)_n$
Hexamethylene diamine	Tier 3 intermediate	Acrylamide	$C_6H_8N_2 + 4H_2 \rightarrow C_6H_{16}N_2$
Bisphenol A	Tier 3 intermediate	Phenol	$2C_6H_6O + C_3H_6O -\rightarrow C_{15}H_{16}O_2$
Methyl methacrylate	Tier 3 intermediate	Acetone	$C_3H_6O + CH_4O + HCN + H_2SO_4 \rightarrow C_5H_8O_2 + NH_4HSO_4$
N-methyl-2-pyrrolidone	Tier 4 intermediate	Gamma-butyrolactone	$C_4H_6O_2 + CH_5N \rightarrow C_5H_9NO + H_2O$
Polycarbonate	End-product	Bisphenol A	$C_{15}H_{16}O_2 + COCl_2 + 2NaOH \rightarrow (C_{16}H_{14}O_3)_n + 2NaCl + 2H_2O$
Polymethyl methacrylate	End-product	Methyl methacrylate	$C_5O_2H_8 \rightarrow (C_5O_2H_8)_n$
Methyl tert-butyl ether	Tier 1 intermediate	Butylenes	$CH_4O + C_4H_8 \rightarrow C_5H_{12}O$
Ethyl tert-butyl ether	Tier 1 intermediate	Butylenes	$C_2H_6O + C_4H_8 \rightarrow C_6H_{14}O$
Polyisobutylene	End-product	Methyl tert-butyl ether	$C_5H_{12}O \rightarrow C_4H_8 + CH_4O$
Polybutadiene	End-product	Butadiene	$C_4H_6 \rightarrow (C_4H_6)_n$

Target chemical	Target category	Starting chemical	Chemical reaction
Nitrobenzene	Tier 1 intermediate	Benzene	$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$
Cyclohexanol / cyclohexanone	Tier 1 intermediate	Benzene	$2C_6H_6 + 5H_2 + O_2 \rightarrow C_6H_{12}O + C_6H_{10}O$
Alkylbenzene	Tier 1 intermediate	Benzene	$C_6H_6 + C_6H_{12} \rightarrow C_{12}H_{18}$
Aniline	Tier 2 intermediate	Nitrobenzene	$C_6H_5NO_2 + H_2 \rightarrow C_6H_7N + O_2$
Adipic acid	Tier 2 intermediate	Cyclohexanol/cyclohexanone	$(C_6H_{12}O + C_6H_{10}O) + HNO_3 \rightarrow 2C_6H_{10}O_4$
Caprolactam	Tier 2 intermediate	Cyclohexanol/cyclohexanone	$(C_6H_{12}O + C_6H_{10}O) + NH_3 \rightarrow 2C_6H_{11}NO + 1.5H_2$
Methylene diphenyl diisocyanate	Tier 3 intermediate	Aniline	$2C_6H_7N + CH_2O + 2COCl_2 \rightarrow C_{15}H_{10}N_2O_2 + 4HCl + H_2O$
Nylon 6	End-product	Caprolactam	$C_6H_{11}NO \rightarrow (C_6H_{11}NO)_n$
Nylon 66	End-product	Hexamethylenediamine	$C_6H_{12}N_2 + C_6H_{10}O_4 \rightarrow (C_{12}H_{22}N_2O_2)_n + H_2O$
Toluene diisocyanate	Tier 1 intermediate	Toluene	$C_7H_8 + 2HNO_3 + 2COCl_2 + 6H_2 \rightarrow C_9H_6N_2O_2 + 6H_2O + 4HCl$
Benzoic acid	Tier 1 intermediate	Toluene	$C_7H_8 + 1.5O_2 \rightarrow C_7H_6O_2 + H_2O$
Sodium / potassium benzoate	Tier 2 intermediate	Benzoic acid	$C_7H_6O_2 + NaOH \rightarrow C_7H_5NaO_2 + H_2O$
Isophthalic acid	Tier 1 intermediate	Meta-xylene	$C_8H_{10} + 3O_2 \rightarrow C_8H_6O_4 + 2H_2O$
Terephthalic acid	Tier 1 intermediate	Para-xylene	$C_8H_{10} + 3O_2 \rightarrow C_8H_6O_4 + 2H_2O$
Dimethyl terephthalate	Tier 1 intermediate	Para-xylene	$C_8H_{10} + 3O_2 + 2CH_4O \rightarrow C_{10}H_{10}O_4 + 4H_2O$
Phthalic anhydride	Tier 1 intermediate	Ortho-xylene	$C_8H_{10} + 3O_2 \rightarrow C_8H_4O_3 + 3H_2O$
Formaldehyde	Tier 1 intermediate	Methanol	$CH_4O \rightarrow CH_2O + H_2$
Acetic acid	Tier 1 intermediate	Methanol	$CH_4O + CO \rightarrow C_2H_4O_2$
Methylamines	Tier 1 intermediate	Methanol	$CH_4O + NH_3 \rightarrow CH_5N + H_2O$
Methyl chloride	Tier 1 intermediate	Methanol	$CH_4O + HCl \rightarrow CH_3Cl + H_2O$
Polyacetal resins	End-product	Formaldehyde	$CH_2O \rightarrow (CH_2O)_n$
Pentaerythritol	Tier 2 intermediate	Formaldehyde	$3CH_2O + C_2H_4O + H_2 \rightarrow C_5H_{12}O_4$
Acetic anhydride	Tier 2 intermediate	Acetic acid	$2C_2H_4O_2 \rightarrow C_4H_6O_3 + H_2O$
Methylene chloride	Tier 2 intermediate	Methyl chloride	$CH_3Cl + Cl_2 \rightarrow CH_2Cl_2 + HCl$
Methyl chlorosilanes	Tier 2 intermediate	Methyl chloride	$2CH_3Cl + Si \rightarrow C_2H_6Cl_2Si$
Cellulose acetates	Tier 3 intermediate	Acetic anhydride	$4C_4H_6O_3 + 4(C_6H_{10}O_5)_n + H_2O \rightarrow C_{20}H_{38}O_{11}$
Chloroform	Tier 3 intermediate	Methylene chloride	$CH_2Cl_2 + Cl_2 \rightarrow CHCl_3 + HCl$
HFC-32	Tier 3 intermediate	Methylene chloride	$CH_2Cl_2 + 2HF \rightarrow CH_2F_2 + 2HCl$
Silicones	Tier 3 intermediate	Methyl chlorosilanes	$C_2H_6Cl_2Si + H_2O \rightarrow (CH_3)_2OSi)_n + 2HCl$
Carbon tetrachloride	Tier 4 intermediate	Chloroform	$CHCl_3 + Cl_2 \rightarrow CCl_4 + HCl$
HCFC-22	Tier 4 intermediate	Chloroform	$CHCl_3 + 2HF \rightarrow CHClF_2 + 2HCl$
Urea	Tier 1 intermediate	Ammonia	$2NH_3 + CO_2 \rightarrow COH_4N_2 + H_2O$
Nitric acid	Tier 1 intermediate	Ammonia	$NH_3 + 2O_2 \rightarrow HNO_3 + H_2O$
Ammonium phosphate	Tier 1 intermediate	Ammonia	$NH_3 + H_3PO_4 \rightarrow NH_4H_2PO_4$
Ammonium sulfate	Tier 1 intermediate	Ammonia	$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$
Hydrogen cyanide	Tier 1 intermediate	Ammonia	$2NH_3 + 2CH_4 + 3O_2 \rightarrow 2HCn + 6H_2O$
Melamine	Tier 2 intermediate	Urea	$6COH_4N_2 \rightarrow C_3H_6N_6 + 6NH_3 + 3CO_2$
Ammonium nitrate	Tier 2 intermediate	Nitric acid	$HNO_3 + NH_3 \rightarrow NH_4NO_3$
Sodium cyanide	Tier 2 intermediate	Hydrogen cyanide	$HCN + NaOH \rightarrow NaCN + H_2O$
Phosgene	Tier 1 intermediate	Chlorine	$CO + Cl_2 \rightarrow COCl_2$
Aluminum chloride	Tier 1 intermediate	Chlorine	$3Cl_2 + Al_2O_3 \rightarrow 2AlCl_3 + 1.5O_2$
Sodium hypochlorite	Tier 1 intermediate	Chlorine	$Cl_2 + 2NaOH \rightarrow NaOCl + NaCl + H_2O$
Calcium hypochlorite	Tier 1 intermediate	Chlorine	$2Cl_2 + 2NaOH + Ca(OH)_2 \rightarrow Ca(OCl)_2 + 2NaCl + 2H_2O$
Titanium dioxide	Tier 1 intermediate	Chlorine	$2Cl_2 + TiO_2 \rightarrow TiO_2 + 2Cl_2$
Aluminum oxide	Tier 1 intermediate	Sodium hydroxide	$NaOH + Al_2O_3 \rightarrow Al_2O_3 + NaOH$
Sodium hydrosulfide	Tier 1 intermediate	Sodium hydroxide	$NaOH + H_2S \rightarrow NaSH + H_2O$
Sodium hydrosulfite	Tier 1 intermediate	Sodium hydroxide	$2NaOH + 2SO_2 \rightarrow Na_2S_2O_4 + O_2$
Sodium sulfide	Tier 1 intermediate	Sodium hydroxide	$2NaOH + 2SO_2 \rightarrow Na_2S_2O_4 + O_2$
Sodium sulfite	Tier 1 intermediate	Sodium hydroxide	$2NaOH + 2SO_2 + Na_2CO_3 \rightarrow 2Na_2SO_3 + CO_2 + H_2O$
Sodium thiosulfate	Tier 1 intermediate	Sodium hydroxide	$2NaOH + 2SO_2 \rightarrow Na_2S_2O_3 + H_2O + O_2$
Aluminum metal	Tier 2 intermediate	Aluminum oxide	$2Al_2O_3 + 3C \rightarrow 4Al + 3CO_2$
Aluminum sulfate	Tier 2 intermediate	Aluminum oxide	$Al_2O_3 + 3H_2SO_4 \rightarrow Al_2(SO_4)_3 + 3H_2O$
Sodium aluminate	Tier 2 intermediate	Aluminum oxide	$Al_2O_3 + 2NaOH \rightarrow 2NaAlO_2 + H_2O$
Phosphoric acid	Tier 1 intermediate	Sulfuric acid	$3H_2SO_4 + Ca_3(PO_4)_2 \rightarrow 2H_3PO_4 + 3CaSO_4$
Hydrofluoric acid	Tier 1 intermediate	Sulfuric acid	$H_2SO_4 + CaF_2 \rightarrow 2HF + CaSO_4$
Glass [e]	End-product	Sodium carbonate	$0.15Na_2CO_3 + 0.75SiO_2 + 0.10CaO \rightarrow (Na_2O)_{0.15}(SiO_2)_{0.75}(CaO)_{0.10} + 0.15CO_2$
Sodium silicate	Tier 1 intermediate	Sodium carbonate	$Na_2CO_3 + SiO_2 \rightarrow Na_2SiO_3 + CO_2$
Sodium bicarbonate	Tier 1 intermediate	Sodium carbonate	$Na_2CO_3 + CO_2 + H_2O \rightarrow SiO_2 + Na_2SO_4 + H_2O$
Silicas	Tier 2 intermediate	Sodium silicate	$Na_2SiO_3 + H_2SO_4 \rightarrow SiO_2 + Na_2SO_4 + H_2O$

[a] Side reaction of: $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$
[b] EVA is typically 15wt% vinyl acetate
[c] EVOH is typically 25-50 mol% ethylene.
[d] Acrylonitrile content varies from 16-53%. 50% assumed here.
[e] Ratio of sodium carbonate, silica, and lime based on ref. [81]

Table S4. Greenhouse gas (GHG) emission factors for the studied chemical classes, where the low and high values are the minimum and maximum of the range of factors sourced from ecoinvent 3.9.1 (with ReCiPe H midpoint method), Carbon Minds, and the Material Flows through Industry tool, in kilogram of carbon dioxide equivalent per kilogram of chemical. Quantity of the chemical class that is wasted each year in the United States (landfill, wastewater treatment, or emission to air, water, or land), in million metric tons (Mt). Total GHG emissions associated with the production of each chemical class for applications that end up being wasted, in Mt carbon dioxide equivalent.

Chemical	GHG emissions, low (kg CO_2 eq./kg)	GHG emissions, high (kg CO_2 eq./kg)	Quantity wasted (Mt)	Wasted GHG emissions, low (Mt CO_2 eq.)	Wasted GHG emissions, high (Mt CO_2 eq.)
Ethylene	0.80	1.93	15.1	12.1	29.1
Propylene	0.95	1.56	6.89	6.55	10.8
Butylenes	1.70	2.39	0.14	0.24	0.33
Benzene	1.23	2.01	2.45	3.01	4.91
Xylenes	1.11	1.84	2.11	2.34	3.88
Toluene	1.00	1.69	0.15	0.15	0.25
Butadiene	1.23	2.37	0.18	0.22	0.43
Ethanol	1.44	3.02	0.31	0.45	0.94
Methanol	0.43	0.93	1.28	0.55	1.19
Sulfuric acid	0.13	0.19	4.93	0.63	0.93
Ammonia	0.51	3.40	8.59	4.38	29.2
Sodium hydroxide	1.18	2.72	4.50	5.31	12.3
Sodium carbonate	0.47	1.33	2.32	1.10	3.07
Chlorine	1.10	2.23	2.95	3.23	6.58

Table S5. Chemicals that are wasted (landfill, wastewater treatment, or emission to air, water, or land) and are listed in the EPA Toxics Release Inventory, as well as their parent chemical and end-product application(s). Human toxicity (carcinogenic and non-carcinogenic) factors for each chemical as calculated from ecoinvent 3.9.1 data and the ReCiPe H endpoint method, in disability adjusted life years (DALYs) per kilogram of chemical. Quantity of each chemical disposed, in million metric tons (Mt), and the total toxicity associated with this waste, in DALYs.

Chemical	Parent chemical	Product type	Proxy chemical	Human toxicity (DALYs / kg)	Quantity disposed (Mt)	Total human toxicity (DALYs)
Acetic anhydride	Methanol	Health care	N/A	1.35E−6	0.020	26.9
Acrylate esters	Propylene	Paper/plastic additives, functional fluids, paint	Butyl acetate	1.55E−6	0.079	122
Acrylic acid	Propylene	Paper/plastic additives, cleaning agents, water treatment	N/A	4.63E−7	0.077	35.4
Acetaldehyde	Ethylene	Personal care	N/A	5.37E−7	0.010	5.4
Ammonia	Ammonia	Crops and food, mining	N/A	6.83E−7	1.32	899
Carbon tetrachloride	Methanol	Functional fluids	N/A	3.85E−7	0.003	1.1
Chlorine	Chlorine	Pulp and paper, water treatment	N/A	4.59E−7	0.68	312
Epichlorohydrin	Propylene	Paints, functional fluids	N/A	1.19E−6	0.012	14.2
Ethanolamine	Ethylene	Mining, cleaning agents, wood laminates, other industrial	N/A	9.22E−7	0.19	173
Ethoxylates	Ethylene	Cleaning agents	Ethoxylated alcohol (AE11)	7.92E−7	0.58	459
Ethylene glycol	Ethylene	Functional fluids	N/A	7.00E−7	0.74	518
Formaldehyde	Methanol	Wood laminates	N/A	4.05E−7	0.04	16.0
HFC-32	Methanol	Functional fluids	Trifluoro-methane	6.48E−6	0.004	30.5
Hydrofluoric acid	Sulfuric acid	Functional fluids, mining	N/A	3.66E−6	0.024	87.8
Isopropanol	Propylene	Solvents, health care	N/A	7.03E−7	0.18	129
Methanol	Methanol	Solvents	N/A	1.69E−7	0.036	6.1
Methyl isobutyl ketone	Propylene	Paper/plastic additives, functional fluids, paints	N/A	1.09E−6	0.009	10.0
Methyl methacrylate	Propylene	Paints	N/A	5.33E−7	0.014	7.4
Methylamine	Methanol	Pulp and paper, water treatment, cleaning agents, other industrial use	N/A	9.02E−7	0.12	106
Methylene chloride	Methanol	Health care, paints	N/A	5.34E−7	0.021	11.1
N-methyl-2-pyrrolidone	Propylene	Paints, solvents	N/A	2.33E−6	0.007	15.7
Nitric acid	Ammonia	Mining	N/A	3.79E−7	0.040	15.2
Phenol	Propylene	Wood laminates	N/A	8.61E−7	0.034	28.9
Phthalic anhydride	Xylenes	Paints,	N/A	5.22E−7	0.002	1.1
Silicones	Methanol	Paper/plastic additives, cleaning agents, functional fluids, health care, paints, personal care	N/A	9.81E−7	0.099	96.7
Sodium cyanide	Ammonia	Mining	N/A	1.28E−6	0.050	64.2
Sulfuric acid	Sulfuric acid	Mining, pulp and paper	N/A	1.14E−6	2.61	2980
Toluene	Toluene	Solvents	N/A	9.09E−8	0.034	3.1

Table S6. Assumptions for the circularity targets and optimistic circularity scenarios.

Product	Relevant chemical class(es)	Circular economy strategy	Measure for circularity targets (M1)	Measure for optimistic circularity (M2)	Justification	Ref.
Antifreeze	Ethylene	Recycle	N/A	80%	M2 assumes the same recycling rate for paint is applicable to antifreeze.	
Food	Ammonia, sulfuric acid	Reduce, Recycle	15% food wasted	10% food wasted, 76% of waste recycled	M1 based on EPA's food waste reduction target. M2 assumes food waste can be further reduced and that overall composting rate can meet that of the food manufacturing and processing sector.	70,82
Glass	Sodium carbonate	Recycle	50%	66%	M1 based on EPA's recycling target. M2 assumes only container and other glass can be recycled with a maximum sorting/recycling yield of 98%.	83,84
HDPE	Ethylene	Recycle	50%	88%	M1 based on EPA's recycling target. M2 based on maximum sorting yield (95%) and mechanical recycling (93%) yield.	83,85
LDPE/ LLDPE	Ethylene	Recycle	50%	90%	M1 based on EPA's recycling target. M2 based on maximum sorting yield (95%) and mechanical recycling yield (95%).	83,85
Nylon 6/66	Propylene, benzene	Recycle	50%	90%	M1 based on EPA's recycling target. M2 based on maximum sorting yield (95%) and chemical recycling yield (95%)	83,86
Other polymers		Recycle	50%	50%	M1 based on EPA's 50% recycling target. M2 assumes no further improvement is possible.	83
Paints and coatings	Ethylene, propylene, methanol, chlorine	Recycle	N/A	80%	M2 assumes that 20% of paint is unrecyclable.	87
PC	Propylene, chlorine	Recycle	50%	50%	M1 based on EPA's 50% recycling target. M2 assumes no further improvement is possible.	83
PET	Ethylene, xylenes	Recycle	50%	95%	M1 based on EPA's recycling target. M2 based on maximum sorting yield (95%) and mechanical recycling yield (90%), with remainder sent to chemical recycling (95% yield).	83,85
PP	Propylene	Recycle	50%	90%	M1 based on EPA's recycling target. M2 based on maximum sorting yield (95%) and mechanical recycling yield (95%).	83,85
PUR	Ethylene, benzene	Recycle	50%	68%	M1 based on EPA's recycling target. M2 assumes that recycling is only applicable to rigid/flexible foams and elastomers (75% of total PUR) with a 90% glycolysis yield.	83,88,89
PVC	Ethylene, chlorine	Recycle	50%	50%	M1 based on EPA's 50% recycling target. M2 assumes no further improvement is possible.	83
Rubbers	Ethylene, butylenes, butadiene, methanol	Recycle	50%	75%	M1 based on EPA's recycling target. M2 assumes a moderate increase in recycling is attainable.	83
Solvents	Propylene, toluene, ethanol, methanol,	Recycle	N/A	85%	M2 assumes that the maximum recycling rate reported for a solvent (N-methylpyrrolidone) in the TRI can be applied to all solvents.	73

Table S7. Disposal of end-of-life chemicals by chemical class and end-product category, in million metric tons (Mt).

	Chemical class (Mt)														
End-product	**Ethylene**	**Propylene**	**Butylenes**	**Benzene**	**Xylenes**	**Toluene**	**Butadiene**	**Ethanol**	**Methanol**	**Sulfuric acid**	**Ammonia**	**Sodium hydroxide**	**Sodium carbonate**	**Chlorine**	**Total**
Adhesives, sealants & functional fluids	1.23	0.49	--	--	--	--	--	--	0.13	0.10	0.01	--	--	--	1.96
Aluminum metal	--	--	--	--	--	--	--	--	--	--	--	1.63	--	--	1.63
Animal feed	0.03	--	--	--	--	--	--	--	0.03	1.68	3.24	--	0.25	--	5.23
Cigarettes	--	--	--	--	--	--	--	--	0.54	0.03	--	--	--	--	0.57
Cleaning agents	0.72	0.06	--	0.16	--	--	--	--	0.10	0.08	--	1.01	0.69	0.51	3.33
Explosives	--	--	--	--	--	--	--	--	--	--	2.21	--	--	--	2.21
Fertilizers	--	--	--	--	--	--	--	--	--	2.05	4.54	--	--	--	6.59
Food	--	--	--	--	--	0.02	--	0.02	--	1.07	2.01	--	0.15	--	3.27
Gasoline	--	0.02	6.02	--	1.30	2.56	--	37.9	0.63	--	--	--	--	--	48.43
Glass	--	--	--	--	--	--	--	--	--	--	--	--	2.64	--	2.64
Health & personal care	0.04	0.40	--	--	--	--	--	0.25	0.12	0.06	--	0.04	0.14	--	1.05
Lead acid batteries			--	--	--	--	--	--	--	0.34	--	--	0.01	--	0.35
Mining & metals	0.04	0.02	--	--	--	--	--	--	--	2.20	0.09	0.11	--	--	2.46
Nylon 6/66	0.03	0.38	--	0.93	--	--	--	--	--	--	--	--	--	--	1.34
Other crops	--	--	--	--	--	--	--	--	--	3.09	5.84	--	--	--	8.93
Other industrial uses	0.32	0.06	--	--	--	--	--	--	0.02	--	--	0.51	0.27	--	1.18
Other polymers	0.58	0.88	--	--	0.14	--	0.05	--	0.23	--	--	--	--	--	1.88
Paints & coatings	0.43	0.83	--	--	0.04	--	--	--	0.05	--	0.02	--	0.04	0.57	1.98
Plastic/paper additives	0.21	0.29	--	--	--	--	--	0.04	0.01	--	--	--	--	0.28	0.83
Polycarbonates	--	0.66	--	--	--	--	--	--	--	--	--	0.23	--	0.37	1.26
Polyethylene, high density	8.54	--	--	--	--	--	--	--	--	--	--	--	--	--	8.54
Polyethylene, low density	10.94	--	--	--	--	--	--	--	--	--	--	--	--	--	10.94
Polyethylene terephthalate	1.54	0.15	--	--	3.16	--	--	--	--	--	--	--	--	--	4.85
Polypropylene	--	7.43	--	--	--	--	--	--	--	--	--	--	--	--	7.43
Polystyrene	0.50	--	--	1.42	--	--	--	--	0.02	--	--	--	--	--	1.94
Polyurethanes	0.84	--	--	1.29	--	0.28	--	--	0.05	--	--	--	--	--	2.46
Polyvinyl chloride	3.13	--	--	--	0.12	--	--	--	--	--	--	--	--	3.84	7.09
Pulp & paper treatment	0.03	--	--	--	--	--	--	--	0.02	0.34	--	2.18	0.12	0.13	2.82
Rubbers	0.49	0.06	0.36	--	--	--	0.35	--	0.20	--	--	--	--	--	1.46
Solvents	--	0.89	--	--	--	0.56	--	0.04	0.46	--	--	--	--	--	1.95
Water treatment	--	0.12	--	--	--	--	--	--	0.04	--	--	1.29	0.05	1.32	2.82
Wood laminates	0.02	0.67	--	--	--	--	--	--	0.79	--	0.66	--	--	--	2.14

Table S8. Disposal of end-of-life chemicals by chemical class and disposal type, in million metric tons (Mt).

Chemical	Longer life (Mt)	Recycling / reuse (Mt)	Energy recover (Mt)	Landfill (Mt)	Wastewater (Mt)	Air emissions (Mt)	Land emissions (Mt)	Water emissions (Mt)	Other (Mt)	Total (Mt)
Ethylene	3.60	1.90	2.70	14.2	0.80	0.00	0.00	0.00	0.50	23.7
Propylene	2.30	0.60	1.50	6.20	0.60	0.10	0.00	0.00	1.30	12.6
Butylenes	0.10	0.20	6.30	0.10	0.00	0.00	0.00	0.00	0.15	6.85
Benzene	0.60	0.10	0.40	2.30	0.15	0.00	0.00	0.00	0.11	3.66
Xylenes	0.30	0.80	2.00	2.10	0.00	0.00	0.00	0.00	0.15	5.35
Toluene	0.10	0.20	2.70	0.10	0.00	0.00	0.00	0.00	0.31	3.41
Butadiene	0.05	0.10	0.10	0.20	0.00	0.00	0.00	0.00	0.00	0.45
Ethanol	0.14	0.04	37.9	0.06	0.24	0.00	0.00	0.00	0.02	38.4
Methanol	0.90	0.37	1.00	0.51	0.28	0.05	0.42	0.02	0.74	4.29
Sulfuric acid	4.52	7.18	0.08	0.13	2.75	0.07	2.72	0.02	1.35	18.8
Ammonia	8.69	2.00	0.20	0.32	0.12	3.04	5.11	0.00	1.51	21.0
Sodium hydroxide	0.49	0.31	0.21	1.16	4.61	0.00	0.00	0.02	0.01	6.81
Sodium carbonate	1.27	0.55	0.23	1.22	0.98	0.00	0.10	0.02	0.35	4.72
Chlorine	2.21	0.82	0.48	1.23	2.01	0.03	0.00	0.01	0.84	7.63
Total	25.3	15.2	55.8	29.8	12.5	3.29	8.35	0.09	7.42	157.7
Ethylene – circularity targets	3.57	9.15	2.65	6.97	0.82	0.00	0.00	0.03	0.51	23.7
Propylene – circularity targets	2.34	3.97	1.54	2.86	0.58	0.07	0.00	0.01	1.17	12.5
Butylenes – circularity targets	0.05	0.27	6.26	0.06	0.00	0.00	0.00	0.00	0.18	6.83
Benzene – circularity targets	0.63	1.38	0.36	1.02	0.16	0.00	0.00	0.00	0.11	3.66
Xylenes – circularity targets	0.33	1.79	1.96	1.08	0.00	0.02	0.00	0.00	0.13	5.32
Toluene – circularity targets	0.08	0.23	2.72	0.06	0.00	0.03	0.00	0.00	0.27	3.39
Butadiene – circularity targets	0.05	0.20	0.10	0.08	0.00	0.00	0.00	0.00	0.02	0.45
Ethanol – circularity targets	0.17	0.04	37.9	0.04	0.24	0.00	0.00	0.01	0.02	38.4
Methanol – circularity targets	0.90	0.55	0.98	0.33	0.28	0.05	0.42	0.02	0.74	4.26
Sulfuric acid – circularity targets	4.69	7.11	0.06	0.07	2.75	0.07	2.71	0.02	1.34	18.8
Ammonia – circularity targets	9.01	1.88	0.17	0.18	0.11	3.04	8.31	0.00	1.50	21.0
Sodium hydroxide – circularity targets	0.49	0.79	0.13	0.77	4.61	0.00	0.00	0.02	0.00	6.81
Sodium carbonate – circularity targets	1.29	1.00	0.23	0.75	0.98	0.00	0.09	0.02	0.36	4.72
Chlorine – circularity targets	2.21	1.46	0.48	0.58	2.01	0.03	0.00	0.01	0.85	7.62
Total – circularity targets	25.8	29.8	55.5	14.8	12.5	3.34	8.31	0.13	7.20	157.5
Ethylene – optimistic circularity	3.57	15.8	0.85	2.15	0.82	0.00	0.00	0.03	0.51	23.7
Propylene – optimistic circularity	2.34	6.93	0.75	1.06	0.58	0.07	0.00	0.01	0.80	12.5
Butylenes – optimistic circularity	0.05	0.35	6.21	0.03	0.00	0.00	0.00	0.00	0.18	6.83
Benzene – optimistic circularity	0.63	2.32	0.11	0.33	0.16	0.00	0.00	0.00	0.11	3.66
Xylenes – optimistic circularity	0.34	3.03	1.63	0.17	0.00	0.02	0.00	0.00	0.13	5.32
Toluene – optimistic circularity	0.08	0.62	2.58	0.04	0.00	0.03	0.00	0.00	0.04	3.39
Butadiene – optimistic circularity	0.05	0.28	0.05	0.05	0.00	0.00	0.00	0.00	0.02	0.45
Ethanol – optimistic circularity	0.18	0.06	37.9	0.03	0.24	0.00	0.00	0.01	0.00	38.4
Methanol – optimistic circularity	0.90	0.90	0.87	0.30	0.28	0.06	0.42	0.02	0.54	4.26
Sulfuric acid – optimistic circularity	4.75	7.12	0.05	0.02	2.75	0.07	2.71	0.02	1.34	18.8
Ammonia – optimistic circularity	9.11	1.91	0.15	0.09	0.11	3.04	5.09	0.00	1.50	21.0
Sodium hydroxide – optimistic circularity	0.48	1.28	0.03	0.31	4.61	0.00	0.00	0.02	0.00	6.73
Sodium carbonate – optimistic circularity	1.30	1.28	0.16	0.53	0.98	0.00	0.09	0.02	0.36	4.72
Chlorine – optimistic circularity	2.21	1.49	0.48	0.55	2.01	0.03	0.00	0.01	0.85	7.62
Total – optimistic circularity	26.0	43.3	51.8	5.66	12.5	3.34	8.31	0.13	6.38	157.4

Table S9. Quantity of the chemical class that is wasted each year in the United States (landfill, wastewater treatment, or emission to air, water, or land) with different circularity scenarios, in million metric tons (Mt). Total greenhouse gas (GHG) emissions associated with the production of each chemical class for applications that end up being wasted, in Mt carbon dioxide equivalent.

	Circularity targets scenario			*Optimistic circularity scenario*		
Chemical	**Quantity wasted (Mt)**	**Wasted GHG emissions, low (Mt CO_2 eq.)**	**Wasted GHG emission, high (Mt CO_2 eq.)**	**Quantity wasted (Mt)**	**Wasted GHG emissions, low (Mt CO_2 eq.)**	**Wasted GHG emission, high (Mt CO_2 eq.)**
Ethylene	7.82	6.26	15.1	3.00	2.40	5.78
Propylene	3.53	3.35	5.52	1.72	1.63	2.69
Butylenes	0.06	0.11	0.15	0.04	0.06	0.09
Benzene	1.18	1.45	2.37	0.49	0.61	0.99
Xylenes	1.11	1.23	2.03	0.20	0.22	0.36
Toluene	0.09	0.09	0.15	0.07	0.07	0.12
Butadiene	0.08	0.09	0.18	0.05	0.06	0.12
Ethanol	0.28	0.40	0.85	0.27	0.40	0.83
Methanol	1.09	0.47	1.02	1.07	0.46	0.99
Sulfuric acid	5.60	0.71	1.05	5.55	0.70	1.04
Ammonia	8.42	4.30	28.6	8.33	4.25	28.3
Sodium hydroxide	4.10	4.84	11.2	3.65	4.30	9.93
Sodium carbonate	1.84	0.87	2.44	1.62	0.77	2.15
Chlorine	1.30	1.43	2.91	1.27	1.40	2.84

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