Supporting Information:

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Supervised life-cycle assessment using automated process inventory based on process recipes

Summary of document details

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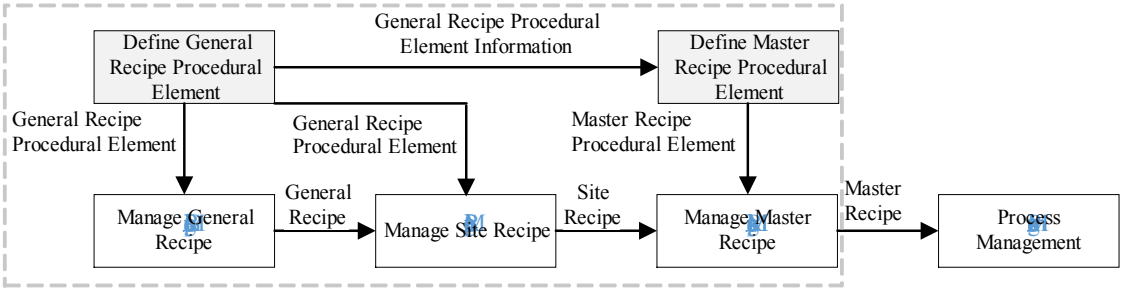

Figure S1. Main control functions in the recipe management.

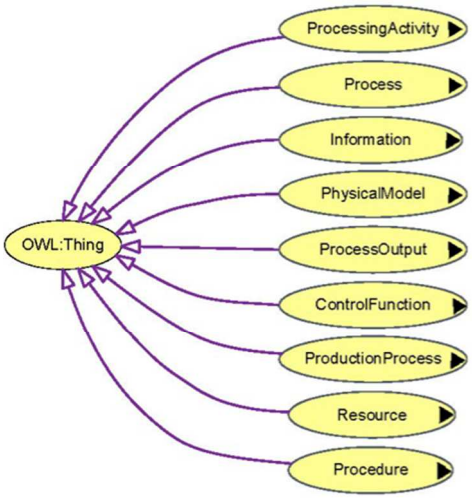

Figure S2. Meta layer of the enterprise ontology project model

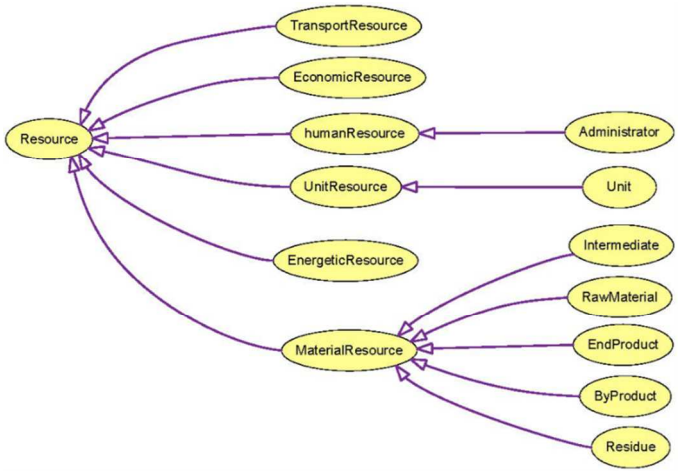

Figure S3. Resource model enterprise ontology project model

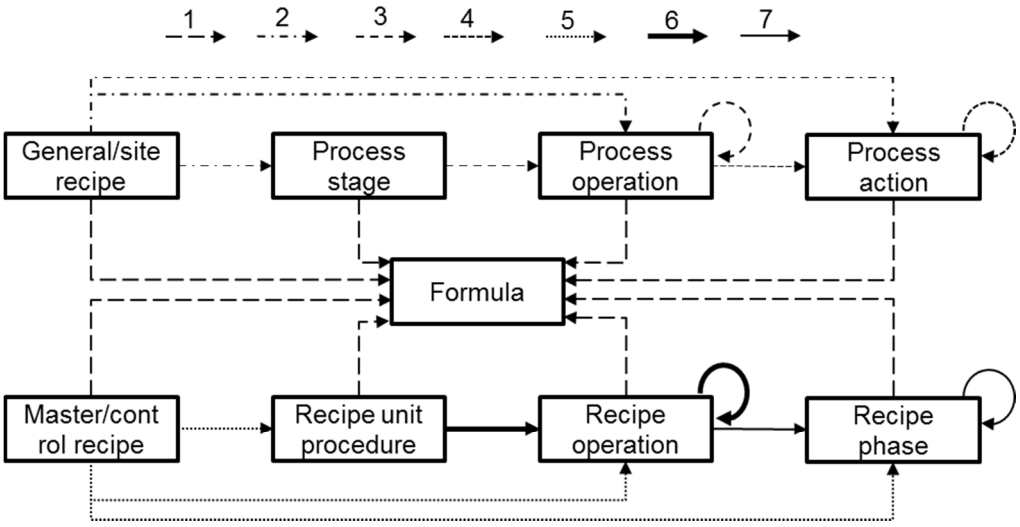

Figure S4. Classes for recipes and recipe procedural elements (rectangles) and their relationships as object properties (arrows: 1. hasFormula; 2. hasProcessModelRecipeProcedure; 3. hasProcessOperation; 4. hasProcessAction; 5. hasProceduralControlModelRecipeProcedure; 6. hasRecipeOperation; 7. has RecipePhase)

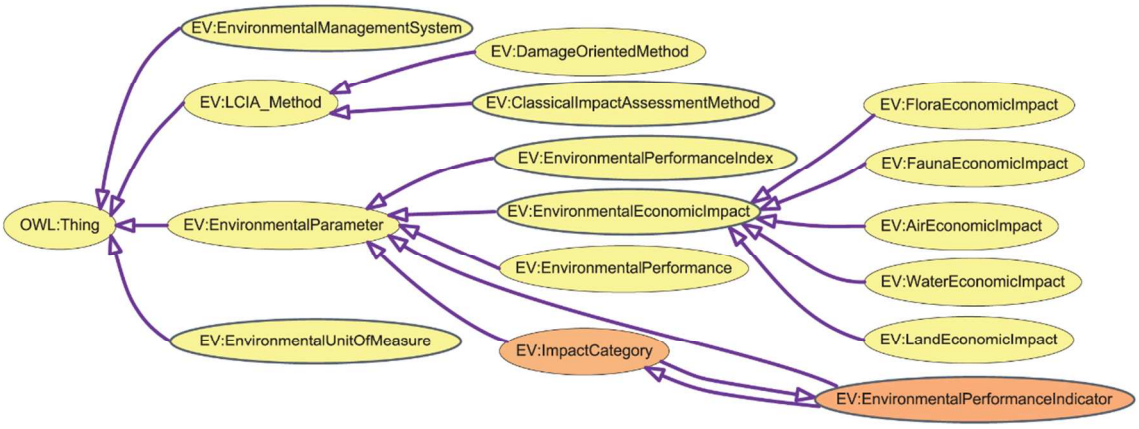

Figure S5. General environmental features within enterprise ontology project model

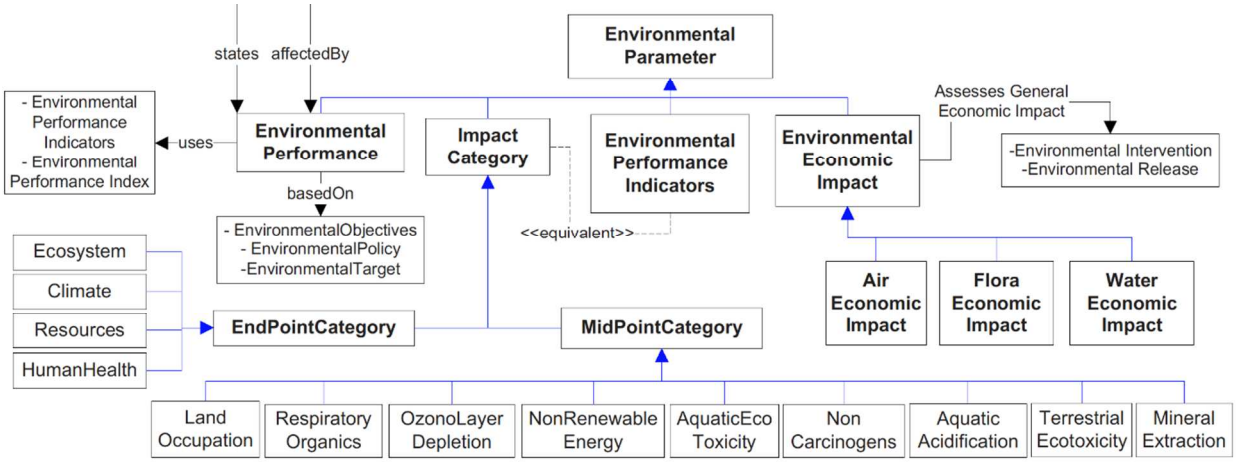

Figure S6. End-point and mid-point impact categories main actors for LCA.

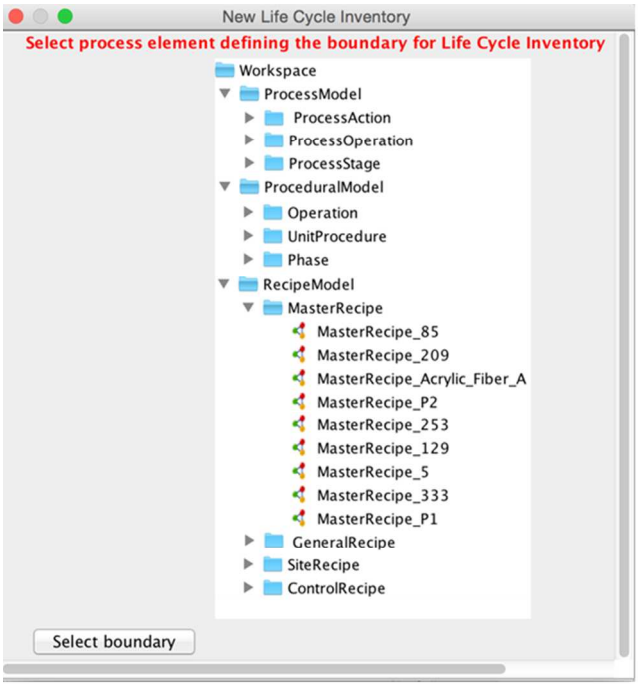

Figure S7. Menu in the framework for selecting the procedural element that defines the boundary for the LCI, expanded over available master recipes.

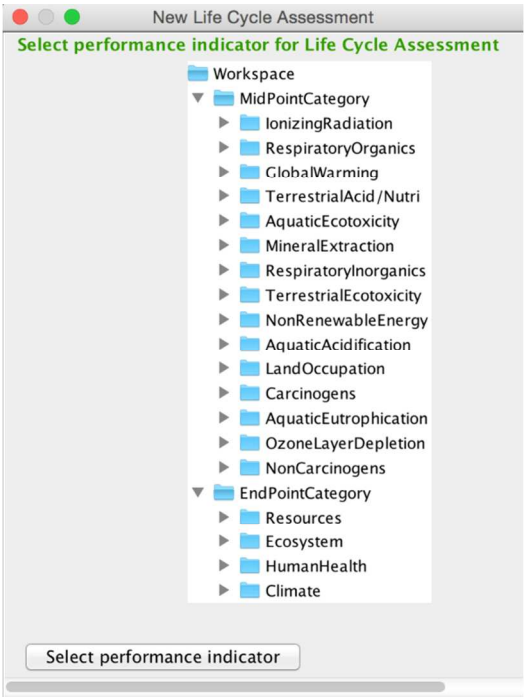

Figure S8. Menu in the framework for selecting the impact categories for implementing the LCA, over the LCI Table.

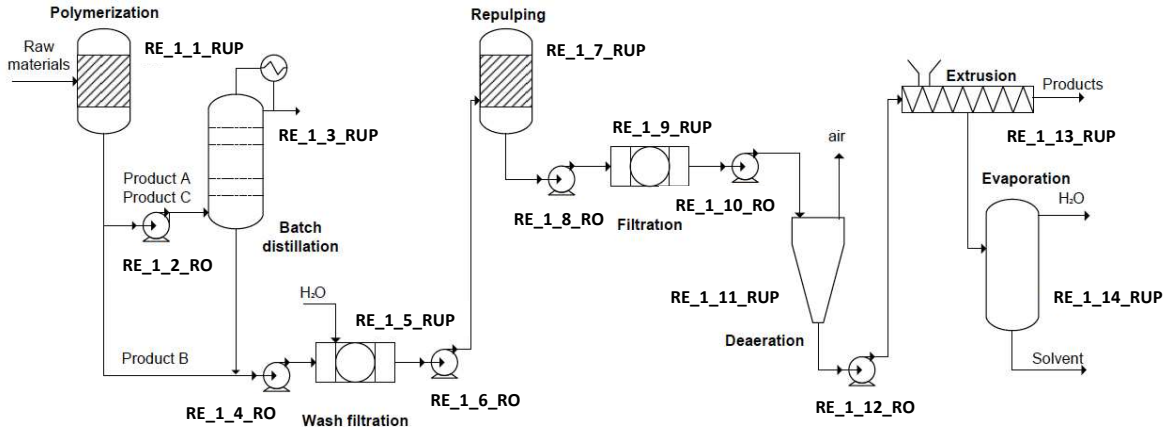

Figure S9. Flowsheet for the production process of acrylic fibers (it contains 14 recipe elements, divided in 8 recipe unit procedures (RUP) and 6 recipe operations (RO).

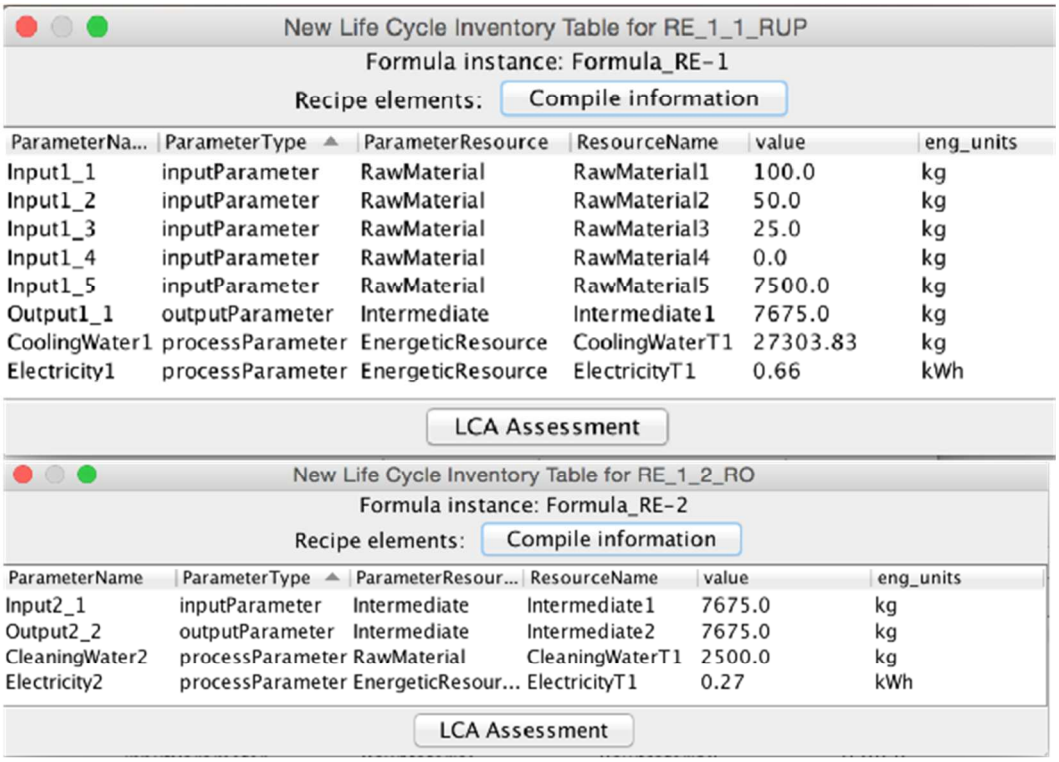

Figure S10. *riTable* for the first two recipe elements (recipe unit procedure and recipe operation) of the master recipe of acrylic fiber A production process.

Additional Tables

Table S1. ANSI/ISA 88 recipe types main features.

Recipe type	Included information	Operation level
General Recipe	Product specific processing information	Procedural
Site Recipe	Site specific information	Procedural
Master Recipe	Process cell, Batch ID, Batch size, In-process-system generated information	Process
Control Recipe	Batch ID, batch size, In-process-system generated information, Timing	Process

Table S2. General and Master Recipe Procedural Elements.

General Procedural Element	Master Procedural Element
Process Action	Recipe Phase
Process Operation	Recipe Operation
Process Stage	Recipe Unit Procedure

Table S3. Enterprise Ontology Project (EOP) general metrics. Regarding model's classes, object properties, data properties, and the description logic expressivity (DL). DLs are used in artificial intelligence to describe and reason about the relevant concepts of an application domain (known as terminological knowledge). This model uses SHIN(D) as DL. Thus, the "S" is the abbreviation for Attributive (Concept) Language with Complements (ALC) with transitive roles; the "H" for rule (property) hierarchy; the "I" for inverse roles; the "N" for the number restrictions (cardinality restrictions, also includes functional properties); and finally the "D" for data-types properties.

Table S3. Enterprise Ontology Project (EOP) general metrics. Regarding model's classes, object properties, data properties, and the description logic expressivity (DL).

Feature	Number/Type
Classes	295
Object properties	257
Data properties	33
Description logic expressivity	SHIN(D)

Table S4. Object and data properties for the class "Parameter".

Object/Data property	Range
hasParameterSource	Resource
hasID_ParameterID	ParameterID
parameter_type	"constant";"variable"
hasEquationAsReferenceValue	MathematicalElement
value	float
engineering_units	string
description	string
scaled	float

Table S5. Object and data properties for the class "Resource" and its subclasses.

Object/Data property	Range
hasID	ResourceID
hasUpperBound/hasLowerBound	float
hasResourceCost	ResourceCost
hasEnvironmentalPerformanceIndex	EnvironmentalPerformanceIndex

Table S6. Object and data properties for the class Environmental Performance Index.

Object/Data property	Range
resultsFromValuation	Valuation
hasImpactCategory	ImpactCategory
describesImpact	EnvironmentalImpact
constant_value	float
engineering_units	string

Table S7. Formula for the master recipe of acrylic fiber A production process.

Parameter Name	Resource Type	Subtype	Resource Name	Procedural Information	Value	Unit
Input1_1	Material	Raw material	Acrylonitrile	Input Parameter	1052.6	kg
Input1_2	Material	Raw material	Methyl Methacrylate	Input Parameter	123.8	kg
Input1_3	Material	Raw material	Vinyl chloride	Input Parameter	61.9	kg
Input1_4	Material	Raw material	Solvent - Acetone	Input Parameter	825.6	kg
Input1_5	Material	Raw material	Styrene	Input Parameter	0.0	kg
Output3_2	Material	Residue	Residue1	Output Parameter	150.0	kg
Output14_1	Material	Residue	Residue2	Output Parameter	103.2	kg
Output14_2	Material	Residue	Residue3	Output Parameter	792.0	kg
Output13_1	Material	Final product	Acrylic Fiber A	Output Parameter	1000.0	kg
Output7_2	Material	Residue	Emissions1	Output Parameter	13.1	kg
Output11_2	Material	Residue	Emissions2	Output Parameter	5.6	kg
CleaningWater_total	Material		CleaningWaterT1	Process Parameter	240000.0	kg
CoolingWater_total	Energetic	Cooling water	CoolingWaterT1	Process Parameter	86139.8	kg
Electricity_total	Energetic	Electricity	ElectricityT1	Process Parameter	4589.4	kWh
Steam_total	Energetic	Steam	SteamP1	Process Parameter	4413.2	kg

Table S8. Formula for the master recipe of acrylic fiber B production process.

Parameter Name	Resource Type	Subtype	Resource Name	Procedural Information	Value	Unit
Input1_1	Material	Raw material	Acrylonitrile	Input Parameter	1052.6	kg
Input1_2	Material	Raw material	Methyl Methacrylate	Input Parameter	123.8	kg
Input1_3	Material	Raw material	Vinyl Chloride	Input Parameter	61.9	kg
Input1_4	Material	Raw material	Solvent - Benzene	Input Parameter	791.8	kg
Input1_5	Material	Raw material	Styrene	Input Parameter	0.0	kg
Output3_2	Material	Residue	Residue1	Output Parameter	155.0	kg
Output14_1	Material	Residue	Residue2	Output Parameter	101.5	kg
Output14_2	Material	Residue	Residue3	Output Parameter	755.4	kg
Output13_1	Material	Final product	Acrylic Fiber B	Output Parameter	1000.0	kg
Output7_2	Material	Residue	Emissions1	Output Parameter	12.9	kg
Output11_2	Material	Residue	Emissions2	Output Parameter	5.3	kg
CleaningWater_total	Material		CleaningWaterT1	Process Parameter	262500.0	kg
CoolingWater_total	Energetic	Cooling water	CoolingWaterT1	Process Parameter	94331.0	kg
Electricity_total	Energetic	Electricity	ElectricityT1	Process Parameter	4854.3	kWh
Steam_total	Energetic	Steam	SteamP1	Process Parameter	5028.1	kg

Table S9. Formula for the complete master recipe of acrylic fiber A production process.

Element ID	Procedural element Type	Parameter Name	Resource Type	Subtype	Resource Name	Procedural Information	Value	Unit
RE-1	Unit procedure	Input1_1	Material	Raw material	Acrylonitrile	Input Parameter	1052.6	kg
RE-1	Unit procedure	Input1_2	Material	Raw material	Methyl Methacrylate	Input Parameter	123.8	kg
RE-1	Unit procedure	Input1_3	Material	Raw material	Vinyl Chloride	Input Parameter	61.9	kg
RE-1	Unit procedure	Input1_4	Material	Raw material	Solvent - Acetone	Input Parameter	825.6	kg
RE-1	Unit procedure	Input1_5	Material	Raw material	Styrene	Input Parameter	0.0	kg
RE-1	Unit procedure	CoolingWater1	Energetic	Cooling water	CoolingWaterT1	Process Parameter	27303.8	kg
RE-1	Unit procedure	Electricity1	Energetic	Electricity	ElectricityT1	Process Parameter	0.7	kWh
RE-1	Unit procedure	Output1_1	Material	Intermediate	Intermediate1	Output Parameter	2064.0	kg
RE-2	Operation	Input2_1	Material	Intermediate	Intermediate1	Input Parameter	2064.0	kg
RE-2	Operation	Output2_1	Material	Intermediate	Intermediate2	Output Parameter	2064.0	kg
RE-2	Operation	Electricity2	Energetic	Electricity	ElectricityT1	Process Parameter	0.3	kWh
RE-2	Operation	CleaningWater2	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-3	Unit procedure	Input3_1	Material	Intermediate	Intermediate2	Input Parameter	2064.0	kg
RE-3	Unit procedure	Output3_1	Material	Intermediate	Intermediate3	Output Parameter	1914.0	kg
RE-3	Unit procedure	Output3_2	Material	Residue	Residue1	Output Parameter	150.0	kg
RE-3	Unit procedure	Electricity3	Energetic	Electricity	ElectricityT1	Input Parameter	883.3	kWh
RE-3	Unit procedure	CoolingWater3	Energetic	Cooling water	CleaningWaterT1	Process Parameter	7500.0	kg
RE-3	Unit procedure	Steam3	Energetic	Steam	SteamP1	Process Parameter	940.1	kg
RE-4	Operation	Input4_1	Material	Intermediate	Intermediate3	Input Parameter	1914.0	kg
RE-4	Operation	Output4_1	Material	Intermediate	Intermediate4	Output Parameter	1914.0	kg
RE-4	Operation	Electricity4	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-4	Operation	CleaningWater4	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-5	Unit procedure	Input5_1	Material	Intermediate	Intermediate4	Input Parameter	1914.0	kg
RE-5	Unit procedure	Output5_1	Material	Intermediate	Intermediate5	Output Parameter	1914.0	kg
RE-5	Unit procedure	Electricity5	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-5	Unit procedure	CleaningWater5	Material	Raw material	CleaningWaterT1	Process Parameter	75000.0	kg
RE-6	Operation	Input6_1	Material	Intermediate	Intermediate5	Input Parameter	1914.0	kg
RE-6	Operation	Output6_1	Material	Intermediate	Intermediate6	Output Parameter	1914.0	kg
RE-6	Operation	Electricity6	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-6	Operation	CleaningWater6	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-7	Unit procedure	Input7_1	Material	Intermediate	Intermediate6	Input Parameter	1914.0	kg
RE-7	Unit procedure	Output7_1	Material	Intermediate	Intermediate7	Output Parameter	1900.9	kg
RE-7	Unit procedure	Output7_2	Material	Residue	Emissions1	Output Parameter	13.1	kg
RE-7	Unit procedure	Electricity7	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-7	Unit procedure	CoolingWater7	Energetic	Cooling water	CoolingWaterT1	Process Parameter	7506.0	kg
RE-8	Operation	Input8_1	Material	Intermediate	Intermediate7	Input Parameter	1900.9	kg
RE-8	Operation	Output8_1	Material	Intermediate	Intermediate8	Output Parameter	1900.9	kg
RE-8	Operation	Electricity8	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-8	Operation	CleaningWater8	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-9	Unit procedure	Input9_1	Material	Intermediate	Intermediate8	Input Parameter	1900.9	kg
RE-9	Unit procedure	Output9_1	Material	Intermediate	Intermediate9	Output Parameter	1900.9	kg
RE-9	Unit procedure	Electricity9	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-9	Unit procedure	CleaningWater9	Material		CleaningWaterT1	Process Parameter	75000.0	kg
RE-10	Operation	Input10_1	Material	Intermediate	Intermediate9	Input Parameter	1900.9	kg
RE-10	Operation	Output10_1	Material	Intermediate	Intermediate10	Output Parameter	1900.9	kg
RE-10	Operation	Electricity10	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-10	Operation	CleaningWater10	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-11	Unit procedure	Input11_1	Material	Intermediate	Intermediate10	Input Parameter	1900.9	kg
RE-11	Unit procedure	Output11_1	Material	Intermediate	Intermediate11	Output Parameter	1895.2	kg
RE-11	Unit procedure	Output11_2	Material	Residue	Emissions2	Output Parameter	5.6	kg
RE-11	Unit procedure	Electricity11	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-11	Unit procedure	CleaningWater11	Material		CleaningWaterT1	Process Parameter	75000.0	kg

RE-12	Operation	Input12_1	Material	Intermediate	Intermediate11	Input Parameter	1895.2	kg
RE-12	Operation	Output12_1	Material	Intermediate	Intermediate12	Output Parameter	1895.2	kg
RE-12	Operation	Electricity12	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-12	Operation	CleaningWater12	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-13	Unit procedure	Input13_1	Material	Intermediate	Intermediate12	Input Parameter	1895.2	kg
RE-13	Unit procedure	Output13_1	Material	Final product	Acrylic Fiber A	Output Parameter	1000.0	kg
RE-13	Unit procedure	Output13_2	Material	Intermediate	Intermediate13	Output Parameter	895.2	kg
RE-13	Unit procedure	Electricity13	Energetic	Electricity	ElectricityT1	Input Parameter	1179.4	kWh
RE-13	Unit procedure	CoolingWater13	Energetic	Cooling water	CoolingWaterT1	Process Parameter	43830.0	kg
RE-13	Unit procedure	Steam13	Energetic	Steam	SteamP1	Process Parameter	1109.3	kg
RE-14	Unit procedure	Input14_1	Material	Intermediate	Intermediate13	Input Parameter	895.2	kg
RE-14	Unit procedure	Output14_1	Material	Residue	Residue2	Output Parameter	103.2	kg
RE-14	Unit procedure	Output14_2	Material	Residue	Residue3	Output Parameter	792.0	kg
RE-14	Unit procedure	Electricity14	Energetic	Electricity	ElectricityT1	Process Parameter	2515.8	kWh
RE-14	Unit procedure	CoolingWater14	Energetic	Cooling water	CoolingWaterT1	Process Parameter	7500.0	kg
RE-14	Unit procedure	Steam14	Energetic	Steam	SteamP1	Process Parameter	2363.8	kg

Table S10. Formula for the complete master recipe of acrylic fiber B production process.

Element ID	Procedural element Type	Parameter Name	Resource Type	Subtype	Resource Name	Procedural Information	Value	Unit
RE-1	Unit procedure	Input1_1	Material	Raw material	Acrylonitrile	Input Parameter	1052.6	kg
RE-1	Unit procedure	Input1_2	Material	Raw material	Methyl Methacrylate	Input Parameter	123.8	kg
RE-1	Unit procedure	Input1_3	Material	Raw material	Vinyl Chloride	Input Parameter	61.9	kg
RE-1	Unit procedure	Input1_4	Material	Raw material	Solvent	Input Parameter	791.8	kg
RE-1	Unit procedure	Input1_5	Material	Raw material	Solvent - Styrene	Input Parameter	0.0	kg
RE-1	Unit procedure	CoolingWater1	Energetic	Cooling water	CoolingWaterT1	Process Parameter	35495.0	kg
RE-1	Unit procedure	Electricity1	Energetic	Electricity	ElectricityT1	Process Parameter	0.7	kWh
RE-1	Unit procedure	Output1_1	Material	Intermediate	Intermediate1	Output Parameter	2030.1	kg
RE-2	Operation	Input2_1	Material	Intermediate	Intermediate1	Input Parameter	2030.1	kg
RE-2	Operation	Output2_1	Material	Intermediate	Intermediate2	Output Parameter	2030.1	kg
RE-2	Operation	Electricity2	Energetic	Electricity	ElectricityT1	Process Parameter	0.3	kWh
RE-2	Operation	CleaningWater2	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-3	Unit procedure	Input3_1	Material	Intermediate	Intermediate2	Input Parameter	2030.1	kg
RE-3	Unit procedure	Output3_1	Material	Intermediate	Intermediate3	Output Parameter	1875.1	kg
RE-3	Unit procedure	Output3_2	Material	Residue	Residue1	Output Parameter	155.0	kg
RE-3	Unit procedure	Electricity3	Energetic	Electricity	ElectricityT1	Input Parameter	1148.3	kWh
RE-3	Unit procedure	CoolingWater3	Energetic	Cooling water	CleaningWaterT1	Process Parameter	7500.0	kg
RE-3	Unit procedure	Steam3	Energetic	Steam	SteamP1	Process Parameter	1222.2	kg
RE-4	Operation	Input4_1	Material	Intermediate	Intermediate3	Input Parameter	1875.1	kg
RE-4	Operation	Output4_1	Material	Intermediate	Intermediate4	Output Parameter	1875.1	kg
RE-4	Operation	Electricity4	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-4	Operation	CleaningWater4	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-5	Unit procedure	Input5_1	Material	Intermediate	Intermediate4	Input Parameter	1875.1	kg
RE-5	Unit procedure	Output5_1	Material	Intermediate	Intermediate5	Output Parameter	1875.1	kg
RE-5	Unit procedure	Electricity5	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-5	Unit procedure	CleaningWater5	Material	Raw material	CleaningWaterT1	Process Parameter	75000.0	kg
RE-6	Operation	Input6_1	Material	Intermediate	Intermediate5	Input Parameter	1875.1	kg
RE-6	Operation	Output6_1	Material	Intermediate	Intermediate6	Output Parameter	1875.1	kg
RE-6	Operation	Electricity6	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-6	Operation	CleaningWater6	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-7	Unit procedure	Input7_1	Material	Intermediate	Intermediate6	Input Parameter	1875.1	kg
RE-7	Unit procedure	Output7_1	Material	Intermediate	Intermediate7	Output Parameter	1862.2	kg
RE-7	Unit procedure	Output7_2	Material	Residue	Emissions1	Output Parameter	12.9	kg
RE-7	Unit procedure	Electricity7	Energetic	Electricity	ElectricityT1	Process Parameter	0.2	kWh
RE-7	Unit procedure	CoolingWater7	Energetic	Cooling water	CoolingWaterT1	Process Parameter	7506.0	kg

RE-8	Operation	Input8_1	Material	Intermediate	Intermediate7	Input Parameter	1862.2	kg
RE-8	Operation	Output8_1	Material	Intermediate	Intermediate8	Output Parameter	1862.2	kg
RE-8	Operation	Electricity8	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-8	Operation	CleaningWater8	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-9	Unit procedure	Input9_1	Material	Intermediate	Intermediate8	Input Parameter	1862.2	kg
RE-9	Unit procedure	Output9_1	Material	Intermediate	Intermediate9	Output Parameter	1862.2	kg
RE-9	Unit procedure	Electricity9	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-9	Unit procedure	CleaningWater9	Material		CleaningWaterT1	Process Parameter	75000.0	kg
RE-10	Operation	Input10_1	Material	Intermediate	Intermediate9	Input Parameter	1862.2	kg
RE-10	Operation	Output10_1	Material	Intermediate	Intermediate10	Output Parameter	1862.2	kg
RE-10	Operation	Electricity10	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-10	Operation	CleaningWater10	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-11	Unit procedure	Input11_1	Material	Intermediate	Intermediate10	Input Parameter	1862.2	kg
RE-11	Unit procedure	Output11_1	Material	Intermediate	Intermediate11	Output Parameter	1856.9	kg
RE-11	Unit procedure	Output11_2	Material	Residue	Emissions2	Output Parameter	5.3	kg
RE-11	Unit procedure	Electricity11	Energetic	Electricity	ElectricityT1	Process Parameter	2.1	kWh
RE-11	Unit procedure	CleaningWater11	Material		CleaningWaterT1	Process Parameter	97500.0	kg
RE-12	Operation	Input12_1	Material	Intermediate	Intermediate11	Input Parameter	1856.9	kg
RE-12	Operation	Output12_1	Material	Intermediate	Intermediate12	Output Parameter	1856.9	kg
RE-12	Operation	Electricity12	Energetic	Electricity	ElectricityT1	Process Parameter	1.2	kWh
RE-12	Operation	CleaningWater12	Material		CleaningWaterT1	Process Parameter	2500.0	kg
RE-13	Unit procedure	Input13_1	Material	Intermediate	Intermediate12	Input Parameter	1856.9	kg
RE-13	Unit procedure	Output13_1	Material	Final product	Acrylic Fiber B	Output Parameter	1000.0	kg
RE-13	Unit procedure	Output13_2	Material	Intermediate	Intermediate13	Output Parameter	856.9	kg
RE-13	Unit procedure	Electricity13	Energetic	Electricity	ElectricityT1	Input Parameter	1179.4	kWh
RE-13	Unit procedure	CoolingWater13	Energetic	Cooling water	CoolingWaterT1	Process Parameter	43830.0	kg
RE-13	Unit procedure	Steam13	Energetic	Steam	SteamP1	Process Parameter	1442.1	kg
RE-14	Unit procedure	Input14_1	Material	Intermediate	Intermediate13	Input Parameter	856.9	kg
RE-14	Unit procedure	Output14_1	Material	Residue	Residue2	Output Parameter	101.5	kg
RE-14	Unit procedure	Output14_2	Material	Residue	Residue3	Output Parameter	755.4	kg
RE-14	Unit procedure	Electricity14	Energetic	Electricity	ElectricityT1	Process Parameter	2515.8	kWh
RE-14	Unit procedure	CoolingWater14	Energetic	Cooling water	CoolingWaterT1	Process Parameter	7500.0	kg
RE-14	Unit procedure	Steam14	Energetic	Steam	SteamP1	Process Parameter	2363.8	kg

Definitions

According to the ISA S88 standard (International Society for Measurement and Control, 1995), the following definitions are provided:

Formula: A piece of recipe information consisting of process inputs, process parameters, and process outputs.

Procedure: The strategy for carrying out a process, namely a major processing action such as making a batch. It is defined in terms of an ordered set of unit procedures.

Unit procedure: An ordered set of operations that causes a contiguous production sequence to take place within a unit. Only one operation is presumed to be active in a unit at any time. An operation is carried to completion in a single unit.

Operation: An ordered set of phases that defines a major processing sequence that takes the material being processed from one state to another, usually involving a chemical or physical change.

Recipe: The necessary set of information that uniquely defines the production requirements for a specific product. There are four different types of recipes, namely general, site, master and control recipes.

Control recipe: A type of recipe which, through its execution, defines the manufacture of a single batch of a specific product.

Master recipe: A type of recipe that accounts for equipment capabilities and may include process cell-specific information.

Recipe operation: An operation that is part of a recipe procedure in a master or control recipe

Recipe unit procedure: A unit procedure that is part of a recipe procedure in a master or control recipe.

Data for the multiproduct batch plant producing acrylic fibers

This section presents the data used for the illustrative case study consisting a multi-product fiber batch plant, which was originally posed in [34].

Plant description and products recipes

The case study consists of a multi-product batch process plant that produces acrylic fiber by a suspension polymerization process requiring 14 processing stages. Due to minimisation of inventory costs, the possible storage of polymer (considered as intermediate product) after stages deaeration (stages 11, 12) has been disregarded and polymer extrusion (stage 13) is performed right after polymer deareation is done. Production recipes contain a detailed description of the product batch sizes [35], operational times and energy demands [35] of each production stage.

Environmental Impact Assessment

Next, the assumptions for calculating the LCI of the products are detailed. Specifically, the data regarding residues, non-controlled emissions, raw materials, steam, water, and electricity consumption are based on good engineering practices and the data available in the literature. Furthermore, the characterization factors of the resources considered in the process recipes are presented in Table S11.

Raw materials consumption estimation. Raw materials (solvent, monomers and initiators) addition for fiber production is considered at stage 1 (polymerization). An overall reaction yield of 95% is assumed. In addition, about 40% of the total initial amount introduced in the reactor is solvent, and the remaining 60% is monomer mixture, which is composed by 85% acrylonitrile, 10% methyl methacrylate and 5% vinyl chloride. The solvent is considered to be pure acetone for production process A and pure benzene for production process B, while vinyl chloride, styrene, acrylonitrile and methyl methacrylate are the possible co-monomers. Each one of the former raw materials LCI data has been retrieved from their corresponding Ecoinvent LCI [36].

Residues generation. The remaining quantity of each batch (about 5% in mass) is released in the last stage (evaporation), and treated as production waste. A certain percentage of consumed water (30%) is also considered as residue to be treated. The LCI associated with its treatment as waste has been related to treatment of "heat carrier liquid, 40% $C_3H_8O_2$, to waste water treatment, class 2/CH S" in Ecoinvent.

Non-controlled emissions. According to US-EPA [37], acrylonitrile emissions in this production process occur at the pelletizer (repulping) and polymer dryer (deaeration) (stages 7 and 11 of the recipe) and estimates an air emission of 18.75 kg/Mg product released in acrylic wet spun homopolymer manufacturing. In this case, these emissions are considered as air emissions of pure acetone, disregarding any monomer emission.

Electricity consumption. Electricity consumption includes pumping required for product movement between stages that are not gravity driven and also for pumping cooling water and steam compression. In the case of pumping cooling water, a pumping $\Delta P=10^5$ Pa and a flow of 20 m^3/h, which requires and approximate power of 1.5 kW, is considered. On the other hand, for compressing heating steam, a yield which represents 0.6 GJ useful heat of steam/GJ electricity is used. In all cases, the LCI information for electricity consumption is considered as "Electricity, medium voltage, at grid/ES U".

Heating and cooling needs. In the case of heating, it is considered to be supplied using steam, the LCI has been gathered using the "Steam, for chemical processes, at plant/RER U" Ecoinvent unit. It is a medium-low pressure saturated steam, at 9 10^5 Pa (2029,45 kJ/kg steam). Steam is used to heat streams according to the recipe provided in [35]. For the estimation of cooling needs, water is used to cool down the streams. All cooling requirements are computed as water cooling and assuming no electrical refrigeration required. Cooling water consumption is computed by taking into account its specific heat (liquid water is 4.18 kJ/kg), and an average ΔT for water of about 20ºC.

Water consumption. Process water is considered to require softening, consequently the Ecoinvent LCI "Water, completely softened, at plant/RER U" is used. Process water is required in some recipe stages besides cooling. The filtering stages require a water flow of 40 m^3/h, and for the cleaning of these units a water flow of 10 m^3/h is needed.

Table S11. Environmental metrics for the different resources in the process recipe.

Resource Name	**Carcinogens [Pt/kg]**	**Global warming [Pt/kg]**
Acrylonitrile	$6.36*10^{-7}$	$5.78*10^{-4}$
Methyl Methacrylate	$6.36*10^{-7}$	$5.78*10^{-4}$
Vinyl Chloride	$1.98*10^{-4}$	$2.49*10^{-4}$
Solvent - Acetone	$2.30*10^{-5}$	$2.01*10^{-4}$
Solvent - Benzene	$7.84*10^{-5}$	$1.46*10^{-4}$
Residue	$1.12*10^{-3}$	$8.16*10^{-2}$
Emissions	0	0
CleaningWaterT1	$2.79*10^{-7}$	$2.04*10^{-5}$
CoolingWaterT1	$3.35*10^{-10}$	$2.37*10^{-9}$
ElectricityT1 [Pt/kWh]	$5.10*10^{-7}$	$5.05*10^{-5}$
SteamP1	$8.19*10^{-7}$	$2.28*10^{-5}$

References

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