

Appendix C: GREENSCOPE

Technical User's Guide

Web-based Version Beta

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Introduction

The GREENSCOPE Web Version software tool allows for quantifying process sustainability with ~140 indicators in four main areas (or bases): Efficiency (26 indicators), Energy (14 indicators), Economics (33 indicators), and Environment (66 indicators). These sets of indicators are capable of transmitting and translating process performance, feedstock, utility, equipment, and output information into a quantifiable sustainability measurement scale. In addition, each indicator is mathematically defined, thus emphasizing realistic usage, and connecting the mathematical formulas for the indicators with their respective data requirements.

GREENSCOPE's methodology has been developed and its software tool designed such that it can be applied to an entire process, to a piece of equipment or process unit, or at the investigatory bench scale. This versatility allows for a direct comparison between several processes manufacturing the same product but employing different raw materials, reaction processes, separation technologies, or producing different byproducts. In addition, the designer or the researcher can implement this methodology to evaluate the sustainability performance either before or after making process modifications. This resulting sustainability assessment describes quantifiably how well the system under consideration makes use of mass and energy inputs to manufacture a valuable product, at the same time meeting social and environmental needs, all the while maximizing its economic benefit.

Users of GREENSCOPE can calculate either all of the indicators available or a desired subset of them. The entire set will provide more complete information, but it is understandable that users could have preferred indicators in which they have more interest. Knowing about the complete list of indicators available can add to understanding of process sustainability, so it is recommended that users read the entire list, even if their focus is on certain indicators.

GREENSCOPE: Web Version

The Web Version of the GREENSCOPE tool contains several toolbars at the landing page that are utilized either for data entries, project library, user profile info, or for indicator calculations.

To get to the project list shown in Figure 1 below one can click "Open an Existing Project" from the My Account page or click "My Projects" at any time on the left of the screen.

The data entry links in "My Projects" page represent:

- Information on various projects is listed here, with links to the indicator types ("Efficiency Indicators", "Environment Indicators", "Energy Indicators", and "Economy Indicators") and to "Show" or "Delete" a project.
- Clicking "Show" allows one to see details about the project, for instance, what libraries are used for compounds, equipment, and/or utilities; reference values; and the number of input and output streams.

The screenshot displays the 'Don's Project List' page. At the top, there's a navigation bar with 'MY ACCOUNT', 'GREENSCOPE', 'TOOLS', and 'SUPPORT'. A sidebar on the left contains a 'My Profile' section with links to 'My Profile', 'My Projects', 'My Compounds', 'My Equipment', 'My Utility Libraries', 'Indicators', and 'Logout'. The main content area is titled 'Don's Projects' and includes a message: 'To Add Anything to The Website Contact dononyx@yahoo.com'. Below this are four buttons: 'Create Project Via Wizard', 'Create Project Advanced', 'Edit User Profile', and 'Logout'. The 'User Projects' section features a table with the following columns: Project Name, Date Modified, Status, Notes, Check Warnings, Efficiency Indicators, Environment Indicators, Energy Indicators, Economy Indicators, Show, and Delete. The table lists several projects, including 'Biodiesel Project', 'My New Project', 'My New ProjectQG', 'My New ProjectQG', 'Ray's test project', 'Text Project', 'Text Wizard Project', and 'My Test Project'.

Figure 1. The Project List page, showing various projects, when they were last modified, any notes about them, and access to parts of the projects through links.

- From the Show page one can click “Edit” to edit various project properties on the Show Project page. This selection will be discussed in detail under 4) below.
- From the Project List page shown in Figure 1, the links to indicator types can be clicked.
- Add Project Stream & Compound Library Data: These features are where input/output stream specifications, reactions, and individual compound properties are localized.
- Create Equipment Library Equipment & Cost Inputs: This link is where equipment specifications, the heat and power demands, and the equipment costs are entered. In addition, some miscellaneous cost inputs are entered here.
- Create Utility Library Data: On this link, utility cost rates, process utility demands, and energy renewability aspects are introduced.

The Indicators calculation link represent:

- Material Efficiency: In this link, the 26 material efficiency indicators are defined and calculated. In addition, each individual indicator is defined conceptually and its mathematic formula, computation algorithm, data inputs, absolute value, best/worst case scenario reference values, and dimensionless score are described and represented. Note that each indicator best and worst case scenario user entries have been defined by

using some default numbers for all indicators. However, users have the option to use other reference values by entry new values in the cells next to the default values. The tool will use the user defined value instead of the default value for the sustainability percent score calculations.

- Environment: The 66 environmental indicators are calculated on this link. These are arranged in the same format as described for the Material Efficiency indicators.
- Energy: The 14 energy indicators are defined, represented, and calculated on this link. Additional calculations for summarizing process heating, cooling, and power needs are described here.
- Economics: The definition, representation, and calculation of the 33 economic indicators are performed on this link. In addition, cash flow analyses and plots for supporting some indicators evaluation are included.
 - Create or Update The Economic Data, Best & Worst-Economics: Since generating or building hypothetical cash flow profiles which are needed for determining the worst and best case economic scenarios is complex, these are provided in a link inside the economic indicator link. These best and worst scenarios were proposed from calculated maximum and minimum average values from current chemical company reports as a function of the manufacturing (COM) and capital (CTM) costs.

In addition, this tool provides a set of databases containing the potency factors of compounds recognized for having negative environmental impacts to the air, soil, and water. These potency factors support the calculation of some environmental indicators (e.g., environmental hazard, air hazard, global warming potential, stratospheric ozone-depletion potential) (this does not require data entries from the user unless the user wants to add data to allow the databases to be more comprehensive).

The successful implementation of the GREENSCOPE sustainability assessment tool, during the conceptual design phase for biodiesel production, has been reported¹ and will be used to detail this software tool and for detailed descriptions throughout this user's guide. The results obtained illustrate the current state of sustainability for the designed simulated biodiesel process and identify possible areas for process improvements, which can lead to increased sustainability for this conceptual process. GREENSCOPE is introduced as a mechanism to assist decision-makers in evaluating and achieving a more sustainable chemical process.

I. Stream & Compound Data Wizards: Step by Step Data Entry Procedure

This data entry page consists of many fill-blank for data entries that are representative of process reference conditions, input streams, chemical reactions, output streams, and individual

compound properties. A step-by-step data entry description to guide the user for entering the required data is described below.

1. Process Temperature and Pressure of Reference

- 1.1. Process reference temperature. This value can be selected from the temperature value (°C) at which the most relevant reaction occurs. If reaction stages are not present in the process, highest process temperature value can be chosen.

Reference temperature and pressure values. These values (temperature in °C and pressure in kPa) are employed for thermodynamic and physicochemical property calculations (e.g., exergy, enthalpy, and entropy). Values of 25 °C and 101.325 kPa are set as default values.

2. DATA ENTRY: Compound, Input, Output Stream Wizards

- 2.1. Compound Name, Molecular Formula, Molecular Weight, and CAS Number. These top blank spaces require entering individual chemical compound data for all chemical substances whether inputs or outputs of the process. The popular chemical compound name (e.g., methanol) is introduced, the simple molecular formula (sequence of elements and number of molecules, e.g., CH₄O) is typed too, the substance's molecular weight [=] kg/kmol (e.g., 32.0419 kg/kmol) is entered in the space below it, and a CAS registry number including dash lines (e.g., 67-56-1) must be entered in a space below the label. This sequence must be implemented for each chemical compound or substance participating in the process (see Figure 2).
- 2.2. Stream number, Feedstock name, and Renewability condition. These stream specifications will help to localize and/or identify data from each feed stream and will be used to evaluate the indicators related to the process inputs (see Figure 2).
- 2.3. Mass flow rates mass flow in kg/hr, for each compound present in each input stream has to be introduced individually. Note that if a compound is a product, its mass flow value in any input stream is zero (see Figure 2).

MY ACCOUNT GREENSCOPE TOOLS SUPPORT

Do Not Create A Compound Already Supplied By Greenscope - You Can Edit The Greenscope Compound Once It Is In Your Compound Library Data Entry Start

If a helper exists, it will be here

Supplied Greenscope Compounds Which Can Be Added To Your Compound Libraries and Edited Later

Ordering	Name	CAS Number	Molecular Weight	Show
All	All	All	All	
6.0	Oil Triolein	122-32-7	885.4320000000	Show
1.0	FAME	112-62-9	296.4880000000	Show
3.0	Methanol	67-56-1	32.0419000000	Show
4.0	Phosphoric Acid	7664-38-2	97.9952000000	Show
5.0	Sodium Phosphate	7801-84-9	163.9410000000	Show
2.0	Glycerol	56-81-5	92.0938000000	Show
7.0	Water	7732-18-5	18.0153000000	Show
8.0	Sodium Hydroxide	1310-73-2	39.9971000000	Show
9.0	Sulfuric Acid	7664-93-9	98.0790000000	Show
10.0	Oleic Acid	112-80-1	282.4800000000	Show
11.0	Sodium Sulphate	7757-82-6	142.0400000000	Show

Compound Name:
Example=> Acetic Acid

Also Known As:
Example=> Ethanoic Acid

CAS Number:
Example=> 64-19-7

Molecular Formula:
Example=> C2H4O2

Molecular Weight:
60.1

What is Compound Used For:
Example=> Feedstock

Start User Compound Creation

Do Not Create A Compound Already Supplied By Greenscope - You Can Edit The Greenscope Compound Once It Is In Your Compound Library Data Entry End, Edit Step Buttons Below.

MY ACCOUNT GREENSCOPE TOOLS SUPPORT

If a helper list exists, it will be here

Input Stream => 103

Project Input Streams

Ordering	Stream Number	Feedstock
All		
1.0	101	Oil-Used
1.0	200	Oil-Used
2.0	102	Methanol
3.0	104	Sodium Hydroxide
4.0	202	Water
5.0	204	Phosphoric Acid
6.0	103	Sulfuric Acid
7.0	106	Glycerol

Stream Number:
103

Feedstock Name:
Sulfuric Acid

Is Renewable:
No

Temperature in C:
25.0000000000
Example => 60.5, if Left Empty Value Will Be 0C.

Pressure in kPa:
100.0000000000
Example => 600, if Left Empty Value Will Be 0kPa.

Vapor Fraction:
0E-10
Example => 0, if Left Empty Value Will Be 0.

Enthalpy in MJ/h:
-80.0630000000
Example => 600, if Left Empty Value Will Be 0MJ/h.

Entropy in MJ/Kh:
-0.0400000000
Example => 600, if Left Empty Value Will Be 0MJ/Kh.

Figure 2. Example of Data inputs for all compounds and material flow streams input to the process or to the system under study.

2.4. Temperature, Pressure, Vapor Fraction stream values. These values have to be collected and entered for each process input stream. Temperature values are to be in Celsius (°C), pressure in kPa, and vapor fraction in terms of mass fraction (see Figure 2).

- 2.5. Enthalpy and Entropy feed stream values. These thermodynamic property values are required in units of MJ/h for enthalpy and MJ/K/h for entropy (see Figure 2).
- 2.6. Feed stream costs. This is the first data input related to cost. Feedstock cost should be accounted per stream instead of individual compound cost. This cost value should be collected for each process input stream (see Figure 2).

3. DATA ENTRY: Reactions

When a reaction occurs within the process, this worksheet (see Figure 3) is the location to introduce relevant reaction data. Individual (net) reaction information must be collected, as well as reaction operating conditions and equipment in which the reaction is performed. Currently, this version of GREENSCOPE can handle multiple individual reactions and several main (global) reactions (e.g., Oil + Methanol \rightarrow Biodiesel + Glycerol), which is the reaction where the main product is obtained (e.g., biodiesel). These reactions are simple reactions occurring under steady state conditions.

- 3.1. Reaction's Stoichiometric Coefficients. The compound stoichiometric coefficients for each chemical reaction must be introduced here. Conventionally, a negative coefficient (e.g., -1, for oil) signifies a reagent and a positive coefficient (e.g., 3 for biodiesel) identifies a product. If a compound does not participate in a specific reaction or is a catalyst (e.g., NaOH), its coefficient is zero (the default value) (see Figure 3).
- 3.2. Main Product and Limiting Reagents. Since a reaction can have multiple products (e.g., biodiesel, glycerol), it is required to specify which of these products (e.g., biodiesel) is the most valuable product or the product of interest. In the same way, the limiting reagent compound (e.g., oil) has to be selected from the group of chemical reagents participating in each reaction (see Figure 3).

The screenshot shows the 'Edit Reaction' interface. At the top, there are navigation tabs: 'MY ACCOUNT', 'GREENSCOPE', 'TOOLS', and 'SUPPORT'. On the left side, there is a helper list with the following items: 'Reaction => Main FAME Reaction', 'Main Global Product => FAME', and 'Main Global Product Stream => 300 FAME'. The main form area contains several input fields:

- Reaction Name For Future Reference:** A text input field containing 'Main FAME Reaction'. Below it, a note states: 'There Can Be Many Valuable Product Reactions In Your Project (Unlike Excel Version That Has 1)'.
- Is Valuable Product Reaction:** A dropdown menu currently set to 'Yes'. Below it, a note states: 'If Yes, Used To Calculate Project Efficiency Indicators'.
- Main Global Reaction Number:** A text input field containing '1'. Below it, a note states: 'You Will Also Have To Enter Reactors For The Main Global Reaction'.
- Main Global Product:** A dropdown menu currently set to 'FAME'. Below it, a note states: 'For This Reaction'.
- Main Global Product Stream:** A dropdown menu currently set to '300 FAME'. Below it, a note states: 'For This Reaction'.

At the bottom of the form, there is a green 'Update' button.

Add Reaction Stoichiometric

MY ACCOUNT GREENSCOPE TOOLS SUPPORT

My Profile

My Projects

My Compounds

My Equipment

My Utility Libraries

Indicators

Logout

Data Entry Start

Compound	Reaction Stoichiometric
FAVE	3.0000000000
Glycerol	1.0000000000
Methanol	-3.0000000000
Phosphoric Acid	
Trisodium Phosphate	
Oil Trislein	-1.0000000000
Water	
Sodium Hydroxide	
Sulfuric Acid	
Oleic Acid	
Sodium Sulphate	

Add Stoichiometrics To Reactor

Data Entry End

Figure 3. Data inputs for all chemical reactions occurring at any process equipment level.

- 3.3. Main Global Reaction Information. These three blank entries collect data required to identify which reaction (e.g., reaction 1) is the one producing the most valuable or desired product (e.g., biodiesel). In addition, the compound number for the main global product (e.g., #1) must be input as well as identifying its corresponding output stream number (e.g., Stream #300) (see Figure 3).
- 3.4. Reaction Equipment and Reaction Operating Conditions. These reaction variables (Temperature °C, Pressure kPa, Enthalpy of reaction MJ/h) and equipment aspects (equipment number) must be input for identifying each reaction's utility needs and for calculation of some safety indicators. In addition, mass fractional conversion of the base component or limiting reagent must be entered here.

4. DATA ENTRY: Output Streams

The last data entries related to process flow streams are the output streams. Data consisting of stream renewability, eco-products, and physical and thermodynamic properties are collected in this group of cells.

- 4.1. Stream Number, Product or Waste Stream Categorization, and Product Name. These stream specifications will be used to localize and/or identify data for each product or output stream as well as evaluation for corresponding sustainability indicators. The Stream number cell and its corresponding number should be entered (e.g., # 300). These stream numbers should be assigned using a three digit series. Currently, the 300 series are used for output streams. For the next cell, a "1" should be selected if this is a product stream or "0" used if it is a waste stream. Finally, if the output stream is a product, a product name should be introduced here in the Product Name cell (see Figure 4).
- 4.2. Eco-product, Pollutant, and Renewability Categorization. The eco-product categorization (only used for product streams) cell needs to be assigned a "1" if the related product stream has eco-product characteristics and a "0" if it does not have any. The non-polluted/polluted categorization (only used for waste streams) cell requires the user to input a "1" if that output waste stream is not-polluted or a "0" if it is polluted. The

renewability categorization (only used only for product streams) cell discriminates whether or not the output product streams is renewable (if so, enter yes) or nonrenewable (then leave blank) (see Figure 4).

- 4.3. Mass Flow Rates. The mass flow rate expressed in kg/hr for each compound present in each output stream has to be introduced individually (see Figure 4).
- 4.4. Temperature, Pressure, Vapor Fraction Stream Values. These values have to be collected and entered for each output process stream. Temperature values should be in Celsius ($^{\circ}\text{C}$), Pressure in kPa, and Vapor fraction in terms mass fraction (see Figure 4).
- 4.5. Enthalpy and Entropy Feed Stream Values. These thermodynamic property values are required in units of MJ/h for enthalpy and MJ/K/h for entropy (see Figure 4).
- 4.6. Output Stream Costs. Product costs should be accounted per stream rather than for each individual compound cost. This cost value should be collected for each product stream (see Figure 4).

Stream Number: 300
Product Name: FAME
Is Product: Yes
Is Eco Product: Yes
Is Polluted: No
Is Hazardous: No
Is Renewable: Yes
Temperature in C: 208.5840000000 Example ==> 25, If Left Empty Value Will Be 0C.
Pressure in kPa: 10.0000000000 Example ==> 25, If Left Empty Value Will Be 0kPa.
Vapor Fraction: 0E-10 Example ==> 25, If Left Empty Value Will Be 0.
Enthalpy in MJ/h: -2007.0000000000 Example ==> 25, If Left Empty Value Will Be 0.

Figure 4. Data inputs for all material flow output streams for the system under study.

5. DATA ENTRY: Compound Properties

This page and its corresponding data are related to the individual or pure compound properties and characteristics. Additionally, there are several categories of data according to a compound's renewability, recyclability and recovery characteristics; solid state properties; chemical safety, exposure and handling; environmental fate; toxicity; classification lists; physical and chemical pure compound properties; thermodynamic properties; and individual potency factors. These pure compound properties are to be aggregated, by mass fraction, in order to estimate the mixture properties for any process stream.

5.1. Mass Input-Output Summary and Categorization.

5.1.1. Waste, Product, Feedstock, Catalyst, Reagent/Solvent, and Other. This category summarizes the material flows of process inputs and outputs for each individual compound. The user is required to categorize each compound as a waste (represented by 0), product (represented by 1), feedstock (represented by 2), catalyst (represented by 3), a feedstock participating as a reagent in the main global reaction and simultaneously acting as a reaction solvent (represented by 4), or other such as drying agent, additive, solvent, washing agent, etc. (represented by 5) (see Figure 5). For category 4 which means a compound is a reagent reacting in the main global reactions but also is a solvent for postreaction purposes, an extra calculation must be performed as described in Efficiency Indicators # 15 and 16. It would be assumed that any amount of excess from the theoretical reaction needs is used as a solvent.

5.2. Renewability, Recyclability, and Recovery.

5.2.1. Renewability Condition. For this data entry, the user must specify if a substance can be categorized as renewable (if yes enter “1”) or nonrenewable (if not enter “0”) material.

5.2.2. Recyclability Condition. This is similar to the previous data entry, where the user can choose if the substance can be recycled within the process or in another process on the site (if yes enter “1”) or not (if not enter “0”) (see Figure 6).

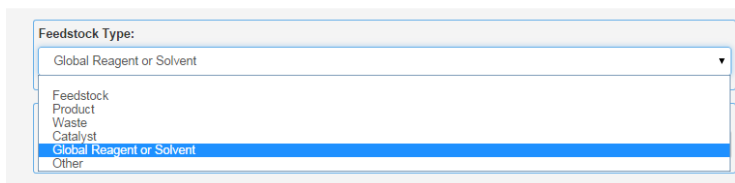
A screenshot of a software interface showing a dropdown menu titled "Feedstock Type:". The menu is open, displaying a list of options: "Global Reagent or Solvent", "Feedstock", "Product", "Waste", "Catalyst", "Global Reagent or Solvent", and "Other". The "Global Reagent or Solvent" option is currently selected and highlighted in blue.

Figure 5. Compound-based categorization for each substance input and output for the system under study.

A screenshot of a software interface showing a vertical stack of seven data entry fields. Each field is a dropdown menu with a downward-pointing arrow on the right side. The fields are labeled as follows: "Is Renewable:", "Is Recyclable:", "Percent of Waste Recovery:", "Is Solid Waste For Landfill:", "Is Solid State:", "Is Solid State at 25C:", and "Is Organic or Water:". The "Percent of Waste Recovery:" field contains the text "0E-10".

Figure 6. Compound-based categorization for renewability, recyclability, and recovery aspects.

5.2.3. Waste Recovery. This data entry requires inserting the percentage amount (based on mass fraction) for each compound present in a non-product output stream that can be recovered for reuse (see Figure 6).

5.3. Solid State.

5.3.1. Some liquid waste can be categorized as solid waste and disposed by way of landfill. The user has to specify if a compound is waste and eligible for landfill disposal (if yes enter “1”) or not (if not enter “0”) (see Figure 6).

5.3.2. Solid State. The user has to specify if a compound is in the solid phase under process operating conditions (if yes enter “1”) or not (if not enter “0”) (see Figure 6).

5.3.3. Organic or Water (aqueous). This last solid state categorization is used to identify organic liquid waste that can be categorized as solid for disposal purposes. The user is required to specify if a compound is organic or water (aqueous) (if yes enter “1”) or not (if not enter “0”) (see Figure 6).

5.4. Chemical Safety, Exposure and Handling

5.4.1. Emergency Response Planning Guidelines (ERPG)-2. The ERPG-2 provides the maximum airborne concentration below which all individuals could be exposed to for up to 1 h without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual’s ability to take protective action, expressed in mg/m³. The “n/a” term is introduced when an ERPG-2 value from a particular compound is unknown (see Figure 7).

ERPG-2 in mg/m3:	OE-10
ERPG-3 in mg/m3:	OE-10
IDLH in mg/m3:	OE-10
MAK in mg/m3:	OE-10
Half Life in Days:	OE-10
OECD 28d in Percent:	OE-10
BCF:	OE-10
Log Kow:	OE-10

Figure 7. Compound-based categorization for chemical safety, exposure and handling, and environmental fate.

5.4.2. ERPG-3. The ERPG-3 in mg/m³, is the maximum airborne concentration below which all individuals could be exposed for up to 1 h without experiencing or developing life-threatening health effects. The “n/a” term is introduced when an ERPG-3 value from a particular compound is unknown (see Figure 7).

5.4.3. Immediately Dangerous to Life and Health (IDLH).² The IDLH in mg/m³, is defined by the US Occupational Safety and Health Administration (OSHA) as an atmosphere that poses an immediate threat to life, would cause irreversible adverse

health effects, or would impair an individual's ability to escape from the dangerous atmosphere. An IDLH value is not necessary when the ERPG-3, EC_{class}, GK, or R-phrase values are known (see Figure 7).

5.4.4. MAK-CH. This data represents the workplace threshold value. This value gives the maximum allowable concentration in air for a chemical substance in the workplace, expressed in mg/m³.

5.5. Environmental Fate

5.5.1. Half-Life. This term defines the degradation half-life (days) for an organic compound. Half-life values for inorganic substances are defined as 0. The user is required to enter either one of two values, half-life or OECD28d (see Figure 7).

5.5.2. OECD28d. This value is the standardized Organization for Economic Cooperation and Development (OECD) method for measuring the biodegradability of organic substances after 28 days, in %. Information regarding the degradability of organic chemicals is used for hazard and risk assessments. As mentioned above in 5.5.1, the user needs to input just one of two values, either half-life or OECD28d (see Figure 7).

5.5.3. Bioconcentration Factor, BCF. The BCF value is the ratio of the concentration of a chemical compound in an organism (e.g., fish) to the concentration of the substance in the surrounding aqueous environment. It is expressed as liter per kilogram (L/kg) (ratio of mass of chemical per kg of organism to mass of chemical per volume of water) (see Figure 7).

5.5.4. Logarithmic Octanol/Water Partitioning Coefficient, K_{ow}.³ This value is the ratio, in a two-phase system of *n*-octanol and water at equilibrium, of the concentration of a chemical substance in the *n*-octanol (organic) phase to that in the water phase (see Figure 7).

5.6. Animal Toxicity

5.6.1. LC₅₀.⁴ This is the lethal dose or amount of substance aqueous concentration that causes 50% mortality of *fathead minnow* after 96 h, mg/L (see Figure 8).

5.6.2. LD₅₀ Oral.³ This is the individual dose administered by oral route required to kill 50% of a population of test animals (e.g., rats), mg/kg (see Figure 8).

5.6.3. LD₅₀ Dermal.³ This is the individual dose administered by dermal (applied to the skin) route required to kill 50% of a population of test animals (e.g., rats), mg/kg (see Figure 8).

5.7. Classification Lists.

5.7.1. Hazardous Classification. For process inputs and outputs, these indicators quantify the potential risk of employed resources or generated compounds, thereby creating an inventory of process hazardous materials. The hazardous material table⁵,

provided by the U.S. Department of Transportation (DOT), can be used as a source to identify hazardous raw materials and output streams (see Figure 9).

The image shows a vertical stack of six input fields on a light gray background. Each field has a label above it and a white input box below it. The labels and their corresponding input values are: 1. 'LC50 in mg/l:' with '0E-10'; 2. 'LC50 Animal Reference and Time:' with an empty box; 3. 'LD50 Oral in mg/kg:' with '0E-10'; 4. 'LD50 Animal Reference and Time:' with an empty box; 5. 'LD50 Dermal in mg/kg:' with '0E-10'; 6. 'LD50 Dermal Animal Reference and Time:' with an empty box. A vertical scrollbar is visible on the right side of the form area.

Figure 8. Compound-based categorization for toxicity effects in animals.

- 5.7.2. The Toxics Release Inventory (TRI) Listed Chemicals.⁶ The purpose of this data entry is to ascertain if a particular chemical used or generated within the process is identified and covered by the TRI Program. These chemicals have been identified to cause cancer or other chronic human health effects, significant adverse acute human health effects, and or significant adverse environmental effects. A “1” is entered when a chemical is listed in the TRI and “0” when it is not listed (see Figure 9).
- 5.7.3. TRI PBT Listed Chemicals.⁷ This is a sub categorization for those substances that possess persistency, bioaccumulative, and toxic (PBT) properties. The TRI program provides a list of PBT chemicals and their chemical compound characteristics. A “1” is input when a chemical is listed on the TRI as a PBT and “0” when it is not listed as a PBT (see Figure 9).
- 5.7.4. European Community (EC) classification Scheme List.⁸ This list is an official classification of identified dangerous substances. This regulatory classification is related to a series of hazard symbols and codes. Some examples are: Harmful substances or preparations (X_n); Flammable substances or preparations classified as extremely flammable (F^+); Toxic substances or preparations classified as toxic (T); Corrosive substances or preparations (C); Irritants (X_i); etc (see Figure 9).
- 5.7.5. Risk Phrase of European Community Codes, R_{code} .⁸ These codes are another classification of substances identified and associated to special risks and danger. Some examples are: Explosive when dry (R1); May cause fire (R7); Toxic by inhalation

(R23). In addition, there are code combinations: Reacts violently with water, liberating extremely flammable gases (R14/15); Very Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed (R39/26/27/28); etc. An R-phrase should be introduced for each compound (see Figure 9).

5.7.6. Swiss Toxicity Classification, GK. This classification for toxic substances is constituted of five different toxicity classes, according to the acute oral lethal dose threshold (LD_{50} oral) as determined on animals (e.g., rats). When a compound GK classification is not described in the Swiss Federal Office of Public Health (SFOPH) database⁹, then the Office bases its classification on the following LD_{50} values: Toxicity class 1: up to 5 mg/kg; Toxicity class 2: 5-50 mg/kg; Toxicity class 3: 50-500 mg/kg; Toxicity class 4: 500-2000 mg/kg; Toxicity class 5: 2000-5000 mg/kg (see Figure 9).

Is Hazardous:	▼
Is On TRI List:	▼
Is On TRI PBT List:	▼
EC Class:	▼
EC Class Approximation:	
R Phrase:	▼
R Phrase Approximation:	
GK:	▼
GK Approximation:	
NFPA Fire Type:	▼

Figure 9. Compound-based categorization by different classification lists.

5.7.7. Flammability Hazard Class, according to the U.S. National Fire Protection Association (NFPA), NFPA-f. According to the NFPA 704 diamond (standard system for the identification of the hazards of materials for emergency response), this system addresses the flammability, health, reactivity, and related hazards by short-term, acute exposure to a material under conditions of fire, spill, or similar emergencies.¹⁰ This is the codification for flammability (diamond red section):

4	Danger	Flammable gas or extremely flammable liquid
3	Warning	Flammable liquid flash point below 100°F
2	Caution	Combustible liquid flash point of 100° to 200°F
1		Combustible if heated
0		Not combustible

5.7.8. Reactivity NFPA-r. These NFPA (-f and -r) data values can be found in many databases.¹¹ This is the codification for reactivity (diamond yellow section):

4	Danger	Explosive material at room temperature
3	Danger	May be explosive if shocked, heated under confinement or mixed with water
2	Warning	Unstable or may react violently if mixed with water
1	Caution	May react if heated or mixed with water but not violently
0	Stable	Not reactive when mixed with water

5.7.9. German Water Hazard Class, WGK (Wassergefährdungsklassen). This legal classification system categorizes substances that are non-hazardous or hazardous to aquatic ecosystems. There are three WGK classes: 1: low hazard to waters; 2: hazard to waters; 3: severe hazard to waters. When a substance is not present in the regulation list or database¹², it is possible to employ the R_{code} values to calculate the WGK classification.¹³ For the purpose of indicator calculation, a compound WGK value is not needed if the LC_{50} is known and provided (see Figure 9).

5.8. Chemical and Physical Properties

- 5.8.1. Pure compound normal boiling point, T_b° . This physical property should be measured at 101.325 kPa and entered in $^\circ\text{C}$ (see Figure 9b).
- 5.8.2. Pure compound normal melting point, T_m° . This physical property should be measured at 101.325 kPa and entered in $^\circ\text{C}$ (see Figure 9b).
- 5.8.3. Flash Point Temperature, T_{flash} . The flash point is a general indication for the flammability or combustibility of a liquid. This physical property should be measured at 101.325 kPa and entered in $^\circ\text{C}$ (see Figure 10). For indicator calculation purposes, a T_{flash} value is not needed if the NFPA-f value is known.

Temperature flash in degree C:
0E-10

-Delta Hc in kJ/kg:
0E-10

Temperature dec in degree C:
0E-10

Delta Hdecom in kJ/kmol(+):
0E-10

Delta Hr in kJ/kg:
0E-10

Figure 10. Compound-based data needs for chemical and physical properties.

- 5.8.4. Combustion Enthalpy, $-\Delta H_C$. This value is the heat generated when a pure compound burns in oxygen under standard thermodynamic conditions. This chemical property should be measured at 101.325 kPa and entered in kJ/kg (see Figure 10).
- 5.8.5. Thermal Decomposition Temperature, T_{dec} . This value is the temperature at which a chemical compound decomposes as the result of breaking chemical bonds. This chemical property should be measured at 101.325 kPa and entered in $^\circ\text{C}$ (see Figure 10). For indicator calculation purposes, a T_{dec} value is not needed if the NFPA-r value is known.
- 5.8.6. Thermal Decomposition Enthalpy, ΔH_{decom} . This endothermic enthalpy is the value required to run a decomposition reaction and should be measured at 101.325 kPa and entered in kJ/kmol (see Figure 10).
- 5.8.7. Reaction Enthalpy, ΔH_r . This enthalpy value is reported in kJ/kg. For indicator calculation purposes, the user has to enter just one of these three values, ΔH_{decom} , ΔH_r , or NFPA-r.

- 5.8.8. Specific Thermal Heat Capacity, C_p° . This value is the amount heat required to change the temperature of one kg of a pure compound by 1 °C. This value should be measured at 101.325 kPa, 25 °C, and entered in kJ/kg/K (see Figure 10).
- 5.8.9. Standard Enthalpy of Vaporization, ΔH_v° . This is the amount of heat required to change a compound from the liquid to gas phase and should be measured at 101.325 kPa, T_b° , and entered in kJ/kg (see Figure 10).

p(rho) in kg/m3:	0E-10
Pv bar:	
pH:	0E-10
Energy Transformity in MseJ/kg:	0E-10
Ex ^{ch} in MJ/kmol:	0E-10
H in MJ/kg with 1 atm and 25 degree C:	-7.2504000000
S in MJ/(kg*K) with 1 atm and 25 degree C:	-0.0064470000

Figure 11. Compound-based data needs for chemical and physical properties (continuation), and for thermodynamic properties.

- 5.8.10. Standard Density, ρ° . A compound's density should be measured at 101.325 kPa, 25 °C, and expressed in kg/m³ units (see Figure 11).
- 5.8.11. Standard Vapor Pressure, P_v° . This is the compound's vapor pressure at thermodynamic equilibrium with its condensed phase (solid or liquid) at 25 °C and 101.325 kPa, expressed in bar units (see Figure 11).
- 5.8.12. pH. This is the measure of the acidity or basicity of an aqueous solution and should be measured at 101.325 kPa and 25 °C (see Figure 11).
- 5.9. Thermodynamic Properties
- 5.9.1. Energy Transformity.¹⁴ This is the amount of energy (the embodied energy required directly and indirectly to produce a good or service) required to produce a given amount of mass or energy of a product (see Figure 11). Transformity values¹⁵ can be expressed as Solar energy Joule (SeJ) per amount of energy, mass, or money (SeJ/J, SeJ/kg, or SeJ/\$, respectively). A lower transformity value means a more efficient conversion step. These are some solar transformity values:

Material or energy type	Transformity, SeJ/J
Sunlight	1
Plant production	6,700
Wood	36,000
Coal	67,000
Oil	90,000
Electricity	300,000

5.9.2. Standard Chemical Exergy, Ex^{och} . Exergy (Ex) is the maximum amount of useful work that can be extracted from a physical system by exchanging mass and energy with the environment (heat transfer process, mass transfer process, chemical reaction, etc.) in a reference state.¹⁶ The chemical exergy accounts for differences in compositions with the environment at standard temperature and pressure. The Ex^{och} value is the reference value¹⁶ for calculating chemical exergy at an ambient temperature of 298.15 K, an atmospheric pressure of 101.325 kPa, and a model of reference species which accounts for the concentration of the most common components of the atmosphere, the oceans and the Earth's crust (see Figure 11). These values are expressed in MJ/kmol

5.9.3. Standard Enthalpy, H° . These values are required to calculate the change of enthalpy flow values for the physical exergy calculation (see section 11.10). This value is calculated at 1 atm and 25 °C. These pure component values can be obtained from a process simulator. The user can create an input-output stream at 25 ° and 1 atm. Then, a 1 kg/h of pure substance i is assumed. This would allow getting the enthalpy and entropy reference values. These values are expressed in MJ/kg (see Figure 11).

5.9.4. Standard Entropy, S° . Similarly to H° , these values are required to calculate the change of entropy flow values for the physical exergy calculation (see section 11.10). This value is calculated at 1 atm and 25 °C. These values are expressed in MJ/kg/K (see Figure 11).

5.10. Potency Factors: Some health, atmospheric, and aquatic effects are quantified by the summation of potency factor (PF) contributions of the different substances. These values are represented as equivalent amounts to a reference substance with a known effect. When values are not input by the user, a value can be found in the internal database by using the compound CAS number.

5.10.1. Benzene Equivalent Potency Factor, $PF_{benzene,i}^F$. These equivalency factor values are employed to assess carcinogenic effects. This value represents the potency factor of the component i as benzene equivalents, kg benzene/kg i (see Figure 12).

5.10.2. Ethylene Equivalent Potency Factor, $PF_{ethylene,i}^F$. These equivalency factor values are employed to assess photochemical oxidation burden. This value represents the

- potency factor of the component *i* as ethylene equivalents, kg ethylene/kg *i* (see Figure 12).
- 5.10.3. Carbon Dioxide Equivalent Potency Factor, $PF_{CO_2,i}$. These equivalency factor values are employed to assess global warming burden. This value represents the potency factor of the component *i* as CO₂ equivalents, kg CO₂/kg *i* (see Figure 12).
- 5.10.4. Sulfur Dioxide Equivalent Potency Factor, $PF_{SO_2,i}$. These equivalency factor values are employed to assess atmospheric acidification burden. This value represents the potency factor of the component *i* as SO₂ equivalents, kg SO₂/kg *i* (see Figure 12).
- 5.10.5. Hydrogen Ion Released Potency Factor, $PF_{H^+,i}$. These potency factor values are employed to assess aquatic acidification burden. This value represents the potency factor of the component *i* as the mass of hydrogen ions released by a unit mass of acid, kg H⁺ /kg *i* (see Figure 12). These PFs are calculated by knowing the total mass or number of hydrogen ions released and divided by its molecular weight.
- 5.10.6. Hydroxide Ion Released Potency Factor, $PF_{OH^-,i}$. These potency factor values are employed to assess aquatic basification burden. This value represents the potency factor of the component *i* as the mass of hydroxide ion released by a unit mass of substance, kg OH⁻ /kg *i* (see Figure 12). These PFs are calculated by knowing the total mass of OH⁻ ions released and divided by the compound molecular weight.
- 5.10.7. Salt-Forming Ion Released. These values account for the number of salt-forming ions (Na⁺, Cl⁻, K⁺, Ca²⁺, Mg²⁺, and SO₄²⁻, PO₄³⁻, etc.) released by a compound (see Figure 12).
- 5.10.8. Salt-Forming Ion Released Molecular Weight. This is the respective molecular weight of the previously identified salt-forming ion released, kg/kmol (see Figure 12).
- 5.10.9. Formaldehyde Equivalent Potency Factor, $PF_{\text{formaldehyde},i}$. These equivalency factor values are employed to assess the ecotoxicity to aquatic life by other substances. This value represents the potency factor of the component *i* as formaldehyde equivalents, kg CH₂O/kg *i* (see Figure 12).
- 5.10.10. Copper Equivalent Potency Factor, $PF_{Cu,i}$. These equivalency factor values are employed to assess the ecotoxicity to aquatic life by metals. This value represents the potency factor of the component *i* as copper equivalents, kg Cu/kg *i* (see Figure 12).
- 5.10.11. Number of Carbon moles, #C. The number of carbon moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.12. Number of Hydrogen moles, #H. The number of hydrogen moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.13. Number of Nitrogen moles, #N. The number of nitrogen moles per unit mole of compound must be entered here (see Figure 12).

- 5.10.14. Number of Chlorine moles, #Cl. The number of chlorine moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.15. Number of Sodium moles, #Na. The number of sodium moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.16. Number of Oxygen moles, #O. The number of oxygen moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.17. Number of Phosphorus moles, #P. The number of phosphorus moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.18. Number of Sulfur moles, #S. The number of sulfur moles per unit mole of compound must be entered here (see Figure 12).
- 5.10.19. Phosphate Equivalent Potency Factor, $PF_{\text{phosphate},i}$. These equivalency factor values are employed to assess eutrophication burden. This value represents the potency factor of the component i as phosphate equivalents, $\text{kg PO}_4^{3-}/\text{kg } i$ (see Figure 12).
- 5.10.20. Trichlorofluoromethane (CFC-11) Equivalent Potency Factor, $PF_{\text{CFC-11},i}$. These equivalency factor values are employed to assess stratospheric ozone-depletion burden. This value represents the potency factor of the component i as CFC-11 equivalents, $\text{kg CFC-11}/\text{kg } i$ (see Figure 12).

Potency Factor, kg benzene/kg i (0 if it is not found):	<input type="text" value="0E-10"/>
Potency Factor, kg ethylene/kg i (0 if it is not found):	<input type="text" value="0E-10"/>
Global Warming Air (kg CO ₂ eq / kg substance):	<input type="text" value="0E-10"/>
Potency Factor, kg SO ₂ /kg i (0 if it is not found):	<input type="text" value="0E-10"/>
Number of H ⁺ ions released:	<input type="text" value="0E-10"/>
PF Acidification water (kg H ⁺ moles eq / kg substance):	<input type="text" value="0E-10"/>
Number of OH ⁻ ions released:	<input type="text" value="0E-10"/>
PF Basification water (kg OH ⁻ moles eq / kg substance):	<input type="text" value="0E-10"/>
Number of salt-forming ions released/compound:	<input type="text" value="0E-10"/>
MW salt-forming ions moles eq in kg/kmol:	<input type="text" value="0E-10"/>

PF salinization water (kg salt-forming ions moles eq / kg substance):

Potency Factor, kg formaldehyde / kg i (0 if it is not found) :

Potency Factor, kg Cu / kg i (0 if it is not found):

Number of Carbon Atoms:

Number of Hydrogen Atoms:

Number of Nitrogen Atoms:

Number of Chlorine Atoms:

Number of Sodium Atoms:

Number of Oxygen Atoms:

Number of Phosphorus Atoms:

Number of Sulfur Atoms:

Eutrophication Water (kg Phosphate eq / kg substance):

Ozone Depletion Air (kg CFC-11 eq / kg substance):

Website Reference:

Ordering For Table Views:

Description of Compound:

Figure 12. Compound-based data needs for potency factors.

II. Equipment & Cost Data Entries: Step by Step data input procedure

This worksheet contains the cells for data for process equipment, miscellaneous costs (e.g., land cost, income tax rate, etc.), feedstock and product costs, etc. Additionally, there are some miscellaneous inputs that can be modified (life of the plant, depreciation method, plant startup time, year in which the first investment is made before the startup time, and present worth factor). All major equipment is considered for cost analysis. Heat and power demands, purchase cost, module cost values are collected from a process cost analysis. In addition, equipment must be categorized when used for waste treatment, solvent recovery, or recycling. For more detailed information regarding equipment cost estimation methods, please see Chapter 7 in Turton et al. (2009).¹⁷

6. Equipment Summary

6.1. Mixers

- 6.1.1. Equipment Number, Equip. #. A 100 series is employed to assign an equipment number. This is followed by a one letter code (e.g., M for mixers, P for pumps, etc.) and completes the equipment numbering process.
- 6.1.2. Equipment name, Name. This entry is optional and not required for any calculation. This data entry can be used as guide to identify some relevant equipment or process steps.
- 6.1.3. Equipment Process Step Classification. This input helps to identify when a particular equipment unit is employed for waste treatment identified by a “1”, solvent recovery identified by a “2”, or for recycling process steps identified by “3”. The “N/A” option is used when the equipment unit does not participate in any one of the above identified categories.
- 6.1.4. Heating or Cooling Needs, Q•. These values are assigned a positive sign “+” if heat is added to the equipment unit or a negative sign “-” if heat is removed (cooling) from the process unit. Values are expressed in terms of MJ/h.
- 6.1.5. Power Needs, Power W•. Identical to heating needs, these values are assigned a positive sign “+” if power is added to the equipment unit or a negative sign “-” if power is generated from the process unit. Values are represented in terms of MJ/h.
- 6.1.6. Total Purchase Cost, \$. This equipment cost provides a value, which is estimated from correlations, which depends on physical variables (e.g., pump purchase cost depends of the shaft power). This is the purchased equipment cost for a base case.
- 6.1.7. Total Module Cost or Installed Cost, \$. This equipment unit cost includes direct, indirect, contingency, and fee costs.
- 6.1.8. Bare Module Cost, \$. This equipment cost represents the summation of direct and indirect costs. For indicator calculation purposes, the equipment summary data requires only one of these costs (Total module costs or bare module costs).

Tie Into Library:	Biodiesel Equipment Library
Type of Equipment:	Distillation Column
Equipment Use:	Recycling
Equipment Name:	Distillation Column 101
Equipment Number:	T-101
Q In Heating Needs:	0E-10 These values are assigned a positive sign + since heat is added to the equipment unit (e.g., distillation column reboiler duty). Values are expressed in terms of MJ/h.
Q In Cooling Needs:	 These values are assigned a negative sign - since heat is removed (cooling) from the equipment unit (e.g., distillation column condenser duty). Values are expressed in terms of MJ/h.
Power In:	0E-10 These values are assigned a positive sign + if power is added to the equipment unit or a negative sign - if power is generated from the process unit. Values are represented in terms of MJ/h.
Total Purchase Cost:	91209.0000000000 This equipment cost provides a value, which is estimated from correlations, which depends on physical variables (e.g., pump purchase cost depends of the shaft power). This is the purchased equipment cost for a base case.
Total Module Cost:	0E-10 This equipment unit cost includes direct, indirect, contingency, and fee costs. For indicator calculation purposes, the equipment summary data requires only one of these costs: Total module costs or bare module costs (next data entry).
Bare Module Cost:	0E-10 This equipment cost represents the summation of direct and indirect costs. For indicator calculation purposes, the equipment summary data requires only one of these costs: Total module costs or bare module costs.
Condenser Duty Cycle - If Applicable:	-369.1245000000
Re-Boiler Duty Cycle - If Applicable:	500.0000000000
Enthalpy Of Reaction - If Applicable:	0E-10
Website Reference:	
Ordering For Table Views:	1.0

Figure 13. Equipment cost data inputs for mixers, pumps, distillation columns, etc.

- 6.2. Pumps. Similar data inputs to that described for mixers (section 6.1) are required for all pumps in the process.
- 6.3. Distillation Columns. Beside the data input requirements for mixers and/or pumps, heating and cooling needs are handled per separation unit. An identified amount of heat must be removed in a condenser and simultaneously an identified amount of heat is added to a reboiler (see Figure 13).
 - 6.3.1. Condenser Duty, MJ/h. This is the amount of excess heat removed to condense the product at the top of the distillation column. In this current version, cooling water is used for all heat removal purposes.
 - 6.3.2. Reboiler Duty, MJ/h. This is the net amount of heat added to a column's reboiler. In this current version, steam is used for all heat addition purposes.
- 6.4. Heat Exchangers, H-100s. Data needs are similar to those for mixers (section 6.1) (see Figure 13).
- 6.5. Extractors, W-100s. Data needs are similar to those for mixers (section 6.1) (see Figure 13).
- 6.6. Component Separators, S-100s. Data needs are similar to those for mixers (section 6.1) (see Figure 13).
- 6.7. Reactors, R-100s. Data needs are similar to those for mixers (section 6.1). In addition, an enthalpy of reaction value is inputted for each reaction system, (MJ/kmol limiting reagent)*(kmol limiting reagent/h) (see Figure 13).
- 6.8. Other Equipment, OE-100s. Data needs are similar to those for mixers (section 6.1) (see Figure 13).
- 6.9. Inventory of Net Energy Consumption for Specific Subprocesses. This subsection summarizes the total amounts of heating, cooling, and electricity demands by equipment involved in waste treatment, (1), solvent recovery (2), and recycling (3). As optional data the unit code names of each equipment unit in the above categories can be entered (see Figure 13).

7. Miscellaneous Data Entries: Water, Costs, FTA

In order to complete some data requirements, other cost parameters must be introduced as well as other process related aspects (see Figure 14).

- 7.1. Liquid water density, kg/m³. This value is required for calculation of water releases and water consumption by the process.
- 7.2. Solid Phase Processing Steps, *P*. This is the number of processing steps involving the handling of particulate solids (e.g., transportation and distribution). If solids are not handled in the process, *P*=0.
- 7.3. Hourly Earnings, \$/h. For estimating the cost of operating labor (*C_{OL}*), the average hourly wage of a chemical plant operator is required. This data can be obtained from

the Bureau of Labor and Statistics (BLS).¹⁸ The BLS reports average hourly earnings of \$27.79 as of December 2010 for employees in the U.S. chemical manufacturing sector. The number of operators per shift is a data requirement; this can be estimated from the equipment required in the Process Flow Diagram (PFD).

- 7.4. Land Cost, C_{land} , \$. This is the investment is made at time zero, decision to establish a plant or process. This is the portion of the fixed capital investment (FCI) that cannot be depreciated.
- 7.5. Salvage Value, rec_m , \$. This is recovered amount from the working capital, land value, and the sale of physical assets evaluated at the end of the plant life (year n). Often this salvage value is neglected.
- 7.6. Discount Rate, r_d . This is the interest rate as an expense of the business operation that is included in the profitability analysis.
- 7.7. Minimum Acceptable Rate of Return, MARR. This is the minimum rate at which the initial investment is recovered in order for it to be acceptable to the investor.¹⁹ This parameter has different values according to the level of risk for the investment: for a low risk project (mature technology process) a MARR value of is 4–8%/yr is used, and for a very high risk investment (unproven technology, high R&D) a MARR value of 32–48%/yr is used.
- 7.8. Fault Tree Assessment, FTA.²⁰ The probability of process failure if the reliability of the individual components is known. This value should be estimated by the user and entry here.

MY ACCOUNT	GREENSCOPE	TOOLS	SUPPORT
Data Entry Start			
If a helper exists, it will be here No Greenscope Supplied Compounds In Library Yet.		<input type="text" value="10.000000000"/> Life of Plant in Years:	
		<input type="text" value="0.300000000"/> Fixed Income Tax Rate in Decimal:	
		<input type="text" value="1.000000000"/> Plant Startup at End of Year:	
		<input type="text" value="1.000000000"/> Year(s) of Investment Before Plant Startup:	
Save and Go To Project Wizard Step 7			
Data Entry End			
Step 1: Project Name And Streams Step 2: Temperature and Pressure Step 3: Steam Pressure and Misc Step 4: Image Uploads Step 5: Water and Costs Step 6: Plant Life and Tax Rate			
Step 7: Salvage Value and Discount Rate Step 8: MARR and FTA Step 9: Libraries Finish Before All Data Entered			
Data Entry End, Edit Step Buttons Below.			

MY ACCOUNT	GREENSCOPE	TOOLS	SUPPORT
Data Entry Start			
If a helper exists, it will be here No Greenscope Supplied Compounds In Library Yet.		<input type="text" value="0E-10"/> Salvage Value of Plant at End of Plant Life:	
		<input type="text" value="0.100000000"/> Discount Rate in Decimal:	
		<input type="text" value="0E-10"/> Discount Rate Best Case in Decimal:	
		<input type="text" value="0.400000000"/> Discount Rate Worst Case in Decimal:	
Save and Go To Project Wizard Step 8			
Data Entry End			
Step 1: Project Name And Streams Step 2: Temperature and Pressure Step 3: Steam Pressure and Misc Step 4: Image Uploads Step 5: Water and Costs Step 6: Plant Life and Tax Rate			
Step 7: Salvage Value and Discount Rate Step 8: MARR and FTA Step 9: Libraries Finish Before All Data Entered			
Data Entry End, Edit Step Buttons Below.			

MY ACCOUNT	GREENSCOPE	TOOLS	SUPPORT
Data Entry Start			
If a helper exists, it will be here No Greenscope Supplied Compounds In Library Yet.		<input type="text" value="0.100000000"/> MARR, Minimum Acceptable Rate of Return in Decimal:	
		<input type="text" value="0.500000000"/> Fault Tree Assessment:	
		<input type="text" value="No"/> Share With The Public:	
		<input type="text" value="No"/> Submit To EPA To Add To Greenscope Library:	
Save and Go To Project Wizard Step 9			
Data Entry End			
Step 1: Project Name And Streams Step 2: Temperature and Pressure Step 3: Steam Pressure and Misc Step 4: Image Uploads Step 5: Water and Costs Step 6: Plant Life and Tax Rate			
Step 7: Salvage Value and Discount Rate Step 8: MARR and FTA Step 9: Libraries Finish Before All Data Entered			
Data Entry End, Edit Step Buttons Below.			

Figure 14. Miscellaneous Data Entries: In order to complete some data requirements, other costs parameters must be introduced as well as other process related aspects.

7.9. Miscellaneous Data Entry: Chemical Exposure Index (CEI)

- 7.9.1. Selected compound for CEI analysis. These data entries are required for evaluating the chemical exposure index (CEI) environmental indicator. The user would select a chemical compound for the CEI analysis. If no compound number is selected the compound with a lower ERPG would be chosen for the CEI analysis.
- 7.9.2. Quantity of liquid available for release, kg. This data entry is the highest hypothetical amount of liquid released in case of fail. By default, a 10 Ton capacity liquid is assumed.
- 7.9.3. Process Stream. This is the stream number having the higher amount of the substance under study for this evaluation.
- 7.9.4. Vapor Pressure at Pool Temperature, kPa. It is assumed the release would happen at standard atmospheric conditions.
- 7.9.5. Diameter of hole, D (mm). A default value of 50.8 mm is assumed in this calculation. The user can overwrite this data entry.
- 7.9.6. Dike area (m^2) and Distance to Property or Fence line (m) values are optional. The indicator evaluation can be more specific when the users can entry these values from their process flow diagrams or safety assessments.

III. Utility Data Entry: Step by Step data input procedure

This data entry page contains the cells to enter the data related to process utilities such as energy inputs (E_k^{in}), water for process use, waste disposal, waste water treatment, air purification, etc. In addition, the renewability nature for energy inputs and energy sources (e.g. steam, cooling water, electricity) are specified here. Utility streams necessary for the process to operate include utilities such as fuel gas, oil, coal, electric power, steam, cooling and process water, boiler feed-water, instrument air, inert gas, and refrigeration.¹⁷ In addition, all utilities provided to the system are expressed as flow rates of mass (e.g., steam) and energy (e.g., electricity) are aggregated by converting to primary fuel equivalent or calorific units. For example, 1 MJ of electricity supplied by either hydroelectric or nuclear is accounted for as equivalent to 3 MJ of the primary energy source used as reference.²¹ The computation of these total utility needs was performed by assuming all utilities are provided off-site and delivered to the battery limit of the modeled process. These assumptions include the following: steam is produced from saturated water at $P = 1.7$ bar and 115 °C using a natural gas-fired industrial boiler with a 90% efficiency that employs 2.251 MJ as a primary energy equivalent (see p. 243 in Turton et al.¹⁷) per kilogram of produced steam. For process cooling needs, moderately low temperature refrigerated water is introduced at 5 °C and returned at 15 °C and is supplied by a combined cooling water loop/refrigeration cycle as described in Turton et al.¹⁷ (pp. 232–238). Additionally, the cooling water is provided off-site and delivered to the process. It is necessary to express these cooling needs in terms of primary energy equivalents (i.e., in this example as

electricity). This value was calculated to be 71.42 kWh of electricity required per 1 GJ of heat removed from the process. In general, 1MJ of electricity is the equivalent of 3 MJ of caloric energy from a primary energy source.²²

8. DATA ENTRY: Utility Costs and Renewability

- 8.1. Utility Cost Rates. Utility costs per unit of energy and mass rates are collected in these cells. Medium pressure steam per unit of mass at 11 bar and 184 °C is employed for utility heat needs. Moderately low temperature refrigerated water ($T_{in} = 5\text{ °C}$ and $T_{out} = 15\text{ °C}$), \$/kg, is employed for utility cooling needs. In addition, electricity is billed or accounted per unit of energy (kWh/h). Steam and cooling water utilities can be billed per GJ of energy added or removed, \$/GJ. In general, the computation of the utility costs can be made assuming that all utilities are provided off-site. For example, Table 8.3 in Turton et al.¹⁷, describes the rates for utilities delivered to the battery limit of a process. The utility cost column has default cost rate values. However, the user can change them for getting a more accurate cost assessment (see Figure 15).
- 8.2. Utility Flow Rate Needs. The amount of utility required by the process is calculated based on the demand of heat energy (e.g., steam cooling water, fuel gas) in equipment such as process heaters, distillation columns, and heat exchangers, or the demand of work (electric power or steam) by compressors, pumps, etc. Generally, the utility flow rates are estimated either by inspection or by doing energy and/or material balances around the equipment. The utility rate needs are calculated automatically. However, extra utility consumption values can be manually entered (see Figure 15).
- 8.3. Liquid Phase Water Type Utility *in situ* Produced. These entries describe those water related utilities (e.g., cooling and process water, boiler feed-water, drinking water, deionized water, etc.) that are produced inside the process under study (“yes”) or provided off-site (“no”) and delivered to the battery limit of the process (see Figure 15).
- 8.4. Renewability for Energy Utility Inputs. A percentage value must be entered here to describe how much energy is supplied by renewable sources (e.g., hydroelectric, wind, solar, etc.) for heating, cooling, and power needs (see Figure 15).

Update a User Utility Library

MY ACCOUNT	GREENSCOPE	TOOLS	SUPPORT	
Utility type	Utility cost, \$US/kg or \$US/kWh	Utility cost, \$US/GJ	Manual Utility flow rate, kg/h	Liq. water util situ
Med pressure steam @10 barg 184°C 1/kg	100.0000000000			
Mod. low T Refrig. water °C Tin = 5 Tout = 15 1/kg	0E-10	0E-10	0E-10	No
Water for process use, cool tower, wash, etc. 1/kg	0E-10	0E-10	0E-10	No
Boiler feed water, 1/kg	0E-10	0E-10	0E-10	No
Potable water, 1/kg	0E-10	0E-10	0E-10	No
Deionized water, 1/kg	0E-10	0E-10	0E-10	No
Electricity (kWh/h)	0E-10	0E-10	0E-10	No
Waste disposal non-Hazard solid 1/kg	0E-10	0E-10	0E-10	No
Waste disposal non-Hazard liquid 1/kg	0E-10	0E-10	0E-10	No
Waste disposal Hazard solid 1/kg	0E-10	0E-10	0E-10	No
Waste disposal Hazard liquid 1/kg	0E-10	0E-10	0E-10	No
Waste water treatment 1st, 1/kg	0E-10	0E-10	0E-10	No
Waste water treatment 2nd, 1/kg	0E-10	0E-10	0E-10	No
Waste water treatment 3rd, 1/kg	0E-10	0E-10	0E-10	No
Air purification, 1/m ³	0E-10	0E-10	0E-10	No
Renewability for energy inputs				
Total % of energy from renewable source	Steam generation 0E-10	Cooling water generation 0E-10	Electricity generation 0E-10	
Steam Energy Source	High Pressure Steam			

Figure 15. The Utility Data tab encloses data requirements for utility demands, utility cost rates, and energy utility renewability.

IV. GREENSCOPE Material Efficiency Indicator Evaluation Page

9. Efficiency Indicators

- The efficiency indicators describe the process sustainability performance in terms of the amount of material and services required to generate the desired product (reaction) or complete a specific process task (e.g., separation). Several indicators are related to unit operation equipment involving chemical reactions, such as classical indicators of chemical reaction efficiency (e.g., reaction yield, atom economy). There are other indicators that employ the total mass or material input to be compared with the product to realize how much mass input is reflected in the product because these values can easily help to quantify the total amount of waste, byproducts, and general releases. Most of the efficiency indicators shown here connect material input/output with the product or service generated in the process or operation unit. More details regarding the efficiency indicators are described in Ruiz-Mercado et al.^{1, 11, 23} A full explanation, mathematical formula, data needs, and worst/best case scenarios for each efficiency indicator will be described below. Please note the current calculations for material efficiency indicators 1, 3, 5, 14, and 16 employ the “main global product flow rate (pure)” value. This is the pure amount of global valuable product (FAME for the biodiesel case study) present in the valuable product stream (stream e.g., Stream # 300) only. For the calculation of other indicators different than the mentioned above, $m_{\text{product}}^{\bullet}$ is the total mass flow rate of the main global product stream.

- Reaction yield, ϵ . Defined as the ratio between actual mass of produced valuable product and the theoretical mass of product that can be generated by assuming all limiting reagent is consumed at all. It is calculated by the ratio between the real yield

(i.e., mass of desired product over the mass of the limiting reagent), over the theoretical yield (i.e., theoretical product flow over the mass of the limiting reagent). The unit is Kg/Kg. Equation (1) describes the calculation of this indicator. Data entries for this indicator are input mass of the limiting reagent ($m_{\text{limit.reagent}}^{\text{in}}$), output mass of product ($m_{\text{product}}^{\bullet}$), reaction's stoichiometric coefficients (β , α), and MW_i . Best case is 1, when the actual yield is same as theoretical yield and worst case 0, when the actual yield is 0 (i.e., the desired products is not formed).

$$\varepsilon = \frac{m_{\text{product}}^{\bullet}}{\frac{m_{\text{limit.reagent}}^{\text{in}}}{MW_{\text{limit.reagent}}} \times \frac{\beta_{\text{product}}}{\alpha_{\text{limit.reagent}}} \times MW_{\text{product}}} \quad (1)$$

9.2. Atom Economy, AE. It is defined as the ratio between the summations of the molecular weight of desired product over the molecular weight of the reactants times their respective stoichiometric coefficients. The unit is kg product/ kg reagents. Equation (2) describes the calculation of this indicator. The reagent and product MW and their stoichiometric coefficients are required data entries. A best case scenario is equal to 1. This is when all the atoms from the reagents are used in the desired product. A worst case value is zero, which means the desired product is not formed.

$$AE_i = \frac{(\beta \times MW)_{\text{product}, i}}{\sum_{i=1}^I (\alpha \times MW)_{\text{reagent}, i}} \quad (2)$$

9.3. Actual Atom Economy, AAE. It is defined as the atom economy when the reaction yield is considered. This is calculated multiplying AE times ε . The unit is kg product/ kg reagents. Equation (3) describes the calculation of this indicator. A value of one is the best case, which is when all the reagent compound atoms are used in the desired product and ε is 100%. A zero value is the worst case scenario.

$$AAE = \frac{(\beta \times MW)_{\text{product}} \times m_{\text{product}}^{\bullet}}{\sum_{i=1}^I (\alpha \times MW)_{\text{reagent}, i} \times \frac{m_{\text{limit.reagent}}^{\text{in}}}{MW_{\text{limit.reagent}}} \times \frac{\beta_{\text{product}}}{\alpha_{\text{limit.reagent}}} \times MW_{\text{product}}} \quad (3)$$

9.4. Stoichiometric Factor, SF. It is an indicator used to quantify the amount of reagents used in excess of the stoichiometric reagent demand described by the limiting reagent. In addition, it can be categorized as a factor to measure the deviation of chemical reaction efficiency from a theoretical 100% efficiency symbolized by stoichiometric mass flow relationships. Equation (4) describes the calculation of this indicator. The

units are actual kg of reagents per kg of theoretical demand of reagents. Best case is 1 (no reagents fed in excess) and worst case is 41 (reagents are 40 times fed in excess to the process).

$$SF = 1 + \frac{\sum_{i=1}^I \left(m_{\text{reagent } i}^{\bullet \text{in}} - \frac{m_{\text{limit. reagent}}^{\bullet \text{in}}}{MW_{\text{limit. reagent}}} \times \frac{\alpha_i}{\alpha_{\text{limit. reagent}}} \times MW_i \right)}{\sum_{i=1}^I \left(\frac{m_{\text{limit. reagent}}^{\bullet \text{in}}}{MW_{\text{limit. reagent}}} \times \frac{\alpha_i}{\alpha_{\text{limit. reagent}}} \times MW_i \right)} \quad (4)$$

9.5. Reaction Mass Efficiency, RME. It is the percentage of the reactants' mass remaining in the desired product. Data entries are desired product mass flow, and total mass flow of the reagents. Equation (5) describes the calculation of this indicator. The unit is kg product / kg reagents. Best case is 1, which is when all mass from the input reagents are converted to the desired product. A worst case value is zero.

$$RME = \frac{m_{\text{product}}^{\bullet}}{\sum m_{\text{reagents}}^{\bullet \text{in}}} \quad (5)$$

9.6. Total material consumption, $m_{\text{mat., tot.}}$. It is the total material inputs of goods and services to the process or process unit. The unit is kg/h. A best case value is when this indicator is equal to the desired product flow rate value. In addition, a worst case value is when this indicator is equal to 40 times the desired product flow rate. Equation (6) describes the calculation of this indicator.

$$m_{\text{mat., tot.}} = \sum_{i=1}^N m_i^{\bullet \text{in}} \quad (6)$$

9.7. Mass intensity, MI. It is the ratio between the total mass fed to the unit over the mass of the desired product. The unit is kg inputs/kg product. A best case equal to 1 is when total inlet mass flow rate is same as the desired product flow rate. A worst case is when total inlet mass flow rate is 40 times the desired product flow rate. Equation (7) describes the calculation of this indicator.

$$MI = \frac{\sum_{i=1}^N m_i^{\bullet \text{in}}}{m_{\text{product}}^{\bullet}} \quad (7)$$

9.8. Value mass intensity, MI_v . It is defined as the ratio between the total mass fed to the process or unit over the total income from product sales. A best case value is 0 and a worst-case score can be suggested using the reference value for MI by selecting a

product whose price is affecting the profitability of the process of interest. For a biodiesel production example, an October 2010 glycerine price is used as the reference product price in determining a worst-case MI_V score equal to 52. Equation (8) describes the calculation of this indicator.

$$MI_V = \frac{\sum_{i=1}^I m_{m,i}^{\bullet \text{in}}}{S_m} \quad (8)$$

9.9. Mass productivity, MP. It is the ratio between the mass of the desired product over the total mass fed. The unit is kg product/kg material inputs. Best case equal to 1 is when all inlet mass is converted to a desired product. Worst case equal to 0 is when desired product is not formed. Equation (9) describes the calculation of this indicator.

$$MP = \frac{m_{\text{product}}^{\bullet}}{\sum_{i=1}^N m_i^{\bullet \text{in}}} \quad (9)$$

9.10. Environmental factor, E . It is the ratio of the mass of waste (without water) per unit of mass of the desired product. A best case equal to 0 is when all inlet mass is converted to main product and no waste produced except water. A worst case equal to 39 is obtained from highest score of average environmental factor values as obtained from the chemical industry. Equation (10) describes the calculation of this indicator.

$$E = \frac{\sum m_{\text{waste} \neq \text{H}_2\text{O}}^{\bullet}}{m_{\text{product}}^{\bullet}} \quad (10)$$

9.11. Mass loss index, MLI. It is the ratio of the mass of waste per unit of mass of valuable product(s). The unit is kg of unconverted mass inputs per kg of valuable product(s). A best case equal to 0 is when all inlet mass is converted to valuable products and no waste is produced. A worst case reference value is 100. Equation (11) describes the calculation of this indicator.

$$MLI = \frac{\sum_{i=1}^N m_i^{\bullet \text{in}} - m_{\text{product}}^{\bullet}}{m_{\text{product}}^{\bullet}} \quad (11)$$

9.12. Environmental factor based on molecular weight, E_{mw} . This is the ratio of the molecular weight of waste per unit of molecular weight of the desired product. The indicator unit results are kg of waste per kg of product. A best case value equal to 0 is

when all inlet mass is converted to main product and no waste. A worst case reference value is 100. Equation (12) describes the calculation of this indicator.

$$E_{mw} = \frac{\sum MW_{waste}}{MW_{product}} \quad (12)$$

9.13. Effective mass yield, EMY. This indicator is defined as the percentage of the mass of desired product relative to the mass of all non-benign materials used in its synthesis. Some substances such as byproducts, reagents or solvents that have no known environmental risk associated with them (i.e., water, low-concentration saline, dilute ethanol, autoclaved cell mass) are considered benign materials. If these 'benign' materials do not enter into the calculations, subjectively EMY is equal to $1/E$. Equation (13) describes the calculation of this indicator. The indicator's result unit is kg of product/ kg hazardous reagents. A zero value in the indicator formula denominator will make the results indeterminate. Therefore, EMY^{-1} is employed to propose the indicator's boundary values. A zero best case value is when all inlet mass is nonhazardous. A worst case scenario value is assumed as 40.

$$EMY = \frac{m_{product}^{\bullet}}{\sum m_{hazardous\ reagents}^{\bullet}} \quad (13)$$

9.14. Carbon efficiency, CE. It is the percentage of carbon in the reactants remaining in the final valuable product. Data entries for this indicator are mass, molecular weight, and number of carbon molecules in the desired product and each component in inlet streams. Equation (14) describes the calculation of this indicator. A best case is 1, which means the number of carbon molecules in the inlet streams is the same as in the desired product. A zero value worst case is when there is no carbon atom in the desired product.

$$CE = \frac{m_{product}^{\bullet} \times (MW_{product})^{-1} \times \text{no. of } C \text{ in product}}{\sum_i^N \left(m_{i, reagent}^{\bullet} (MW_{i, reagent})^{-1} \times \text{no. of } C \text{ in } i \right)} \quad (14)$$

9.15. Material Recovery Parameter, MRP. This indicator assesses all material used in reaction and separation operation units and subprocesses such as reaction and separation solvents, catalysts, additives, and drying agents. It indicates the amount of these materials, which are recovered or eliminated per mass material used. Data entries for this indicator are total input of solvent and catalyst and total solvent and catalyst recovered. The unit is kg recovered material/ kg used material. Equation (15)

describes the calculation of this indicator. A best case value equal to 1 is when all purification, solvents, and catalyst materials are recovered, recycled, and/or eliminated. A worst case value equal to 0 is when purification, solvents, and catalyst materials are not recovered, recycled, and/or eliminated. When a compound is a reagent reacting in the main global reactions but also is a solvent for postreaction purposes (classification #4), an extra calculation must be performed. It would assumed that any amount of excess from the theoretical reaction needs is used as a solvent. This is calculated by this way:

$$m_{\text{solvent}, i}^{\bullet \text{in}} = m_{\text{reagent/solvent}, i}^{\bullet \text{in}} - \frac{m_{\text{limit. reagent}}^{\bullet \text{in}}}{\text{MW}_{\text{limit. reagent}}} \times \frac{\alpha_{\text{reagent}, i}}{\alpha_{\text{limit. reagent}}} \times \text{MW}_{\text{reagent}, i}$$

Where $m_{\text{solvent}, i}^{\bullet \text{in}}$ is the total input amount of substance i classified as 4 that is used mainly as a solvent, $m_{\text{reagent/solvent}, i}^{\bullet \text{in}}$ is the total mass input of substance i classified as 4, and $\alpha_{\text{reagent}, i}$ is the stoichiometric coefficient of substance i in the main global reaction.

$$\text{MRP} = \frac{\sum \left(m_{\text{solvent}}^{\bullet \text{reaction}} + m_{\text{solvent}}^{\bullet \text{postreaction}} + m_{\text{catalyst}}^{\bullet \text{reaction}} + m_{\text{catalyst}}^{\bullet \text{postreaction}} \right)_{\text{recovered}}}{\sum \left(m_{\text{solvent}}^{\bullet \text{reaction}} + m_{\text{solvent}}^{\bullet \text{postreaction}} + m_{\text{catalyst}}^{\bullet \text{reaction}} + m_{\text{catalyst}}^{\bullet \text{postreaction}} \right)_{\text{used}}} \quad (15)$$

9.16. Solvent and catalyst environmental impact parameter, f . This indicator describes the amount of solvents and materials, and mass of catalysts employed on reaction and post reaction operating units per mass of collected desired product. Equation (16) describes the calculation of this indicator. A best case scenario value of 0 is when all purification, solvents, and catalyst materials are recovered, recycled, and/or eliminated. A worst case value is 62.²³

$$f = \frac{\sum \left(m_{\text{solvent}}^{\bullet \text{reaction}} + m_{\text{solvent}}^{\bullet \text{postreaction}} + m_{\text{Catalyst}}^{\bullet \text{reaction}} + m_{\text{Catalyst}}^{\bullet \text{postreaction}} \right)}{m_{\text{product}}^{\bullet}} \quad (16)$$

9.17. Physical return on investment, pROI_M . This represents the ratio of the value of product and byproduct to the extra quantity of resources needed to convert the raw materials into the product(s) and byproduct(s). Data entries are desired product and byproduct mass flows and total mass flow in. Equation (17) describes the calculation of this indicator. A zero value in the indicator formula denominator will make the results indeterminate. Therefore, a pROI_M^{-1} is employed to propose the indicator's boundary values. A best case inverse value of 0 is when all inlet mass is converted to product and byproduct and no waste is produced. A worst case inverse value is 40.²³

$$\text{pROI}_M = \frac{m_{\text{product}}^{\bullet}}{\sum_{i=1}^N m_i^{\bullet \text{in}} - m_{\text{product}}^{\bullet}} \quad (17)$$

9.18. Renewability-material index, RI_M . This is the fraction of the total consumed feedstocks categorized as renewable resources. It lies between 0 and 1. Data entries for its calculation include the renewable material list and the process input mass flows. Equation (18) describes the calculation of this indicator. A best case is 1, which means that all inlet mass is renewable. Worst case is 0 or when no inlet mass is renewable.

$$\text{RI}_M = \frac{\sum_{i=1}^{N_r} (m_i^{\bullet \text{in}})_{\text{renewable}}}{\sum_{i=1}^N m_i^{\bullet \text{in}}} \quad (18)$$

9.19. Breeding-material factor, BF_M . This indicator represents a proportional ratio between the total mass input to the process to the nonrenewable mass inputs. Equation (19) describes the calculation of this indicator. A best case value corresponding to 10 is when all inlet mass is 10 times the value of the total nonrenewable inlet mass and a worst case is 0.

$$\text{BF}_M = \frac{\sum_{i=1}^N m_i^{\bullet \text{in}}}{\left(\sum_{i=1}^N m_i^{\bullet \text{in}} - \sum_{i=1}^{N_r} (m_i^{\bullet \text{in}})_{\text{renewable}} \right)} \quad (19)$$

9.20. Recycled material fraction, $w_{\text{recycl. mat.}}$. This is the fraction of the total consumed feedstocks categorized or identified as recyclable material. It lies between 0 and 1. Data entries for its calculation include the recyclable material list and the process input mass flows. Equation (20) describes the calculation of this indicator. Best case is 1 or when all material process inputs were recycled. A worst case value of 0 is when no material inputs are non-recycled materials.

$$w_{\text{recycl. mat.}} = \frac{\sum_{i=1}^{N'} (m_i^{\bullet \text{in}})_{\text{recyclable}}}{\sum_{i=1}^N m_i^{\bullet \text{in}}} \quad (20)$$

9.21. Mass fraction of products from recyclable materials, $w_{\text{recycl. prod.}}$. This is the amount (fraction) of the mass of valuable products derived from recyclable material inputs. Equation (21) describes the calculation of this indicator. A best case value of 1

is when all material inputs are from recycled materials and 1 kg of valuable product is created from 1 kg of feedstocks (recycled). A worst case of 0 is when no inlet mass is from recycled materials.

$$W_{\text{recycl. prod.}} = \frac{\sum_{i=1}^N (m_{\text{reagent } i}^{\bullet \text{in}})_{\text{recyclable}}}{m_{\text{product}}^{\bullet}} \quad (21)$$

9.22. Mass fraction of products designed for disassembly, reuse or recycling, $w_{\text{recov. prod.}}$. This indicator assesses the fraction of valuable product(s) that can be recovered for reuse or recycling. Equation (22) describes the calculation of this indicator. A best case value of 1 means all products after their use can be disassembled, reused, or recycled. A worst case value is 0.

$$W_{\text{recov. prod.}} = \frac{\sum_{i=1}^M (m_{\text{product } i}^{\bullet})_{\text{recyclable}}}{\sum_{i=1}^M m_{\text{product } i}^{\bullet}} \quad (22)$$

9.23. Total water consumption, $V_{\text{water, tot.}}$. This indicator assesses the total volume of water consumed in the process. This assessment (excluding rainwater) can include evaporation and misting losses from cooling water, water vapor vented to the atmosphere, water lost through waste treatment or disposal, and water lost through deep-well injection. Equation (23) describes the calculation of this indicator. Data entries are water flow inputs and recovered water flow rates. The indicator's results are in unit is m^3 water/h. A best case of 0 is when all water used into the process is recovered, reused, or recycled. A worst case is when no water is recovered.

$$V_{\text{water, tot.}} = \frac{1}{\rho_{\text{H}_2\text{O}}} \left(\sum_{i=1}^N m_{\text{H}_2\text{O } i}^{\bullet \text{in}} - m_{\text{H}_2\text{O}}^{\bullet \text{recovered}} \right) \quad (23)$$

9.24. Fractional water consumption, FWC. This the amount of water consumed (m^3/h) by the manufacturing process per unit mass of valuable product(s) (kg/h). Equation (24) describes the calculation of this indicator. A best case is 0 or when all water is recovered (except water content in the valuable products). A worst case value is 2.95.²³

$$\text{FWC} = \frac{1}{\rho_{\text{H}_2\text{O}} m_{\text{product}}^{\bullet}} \sum_{i=1}^N m_{\text{H}_2\text{O } i}^{\bullet \text{in}} \quad (24)$$

9.25. Water intensity, WI. This the amount of water consumed (m³/h) by the manufacturing process per sales revenue from valuable product(s) (\$/h). Equation (25) describes the calculation of this indicator. A best case is 0 or when no fresh water is fed to the process. A worst case is 1.55.²³

$$WI = \frac{Q_{H2O}^{in}}{S_{product}} \quad (25)$$

9.26. Volume fraction of water type, $\phi_{water\ type}$. This is determined for all types of water or rather quality of the consumed water, such as drinking water and raw water (surface, well, lake, river, or rain water). Equation (26) describes the calculation of this indicator. Data entries for this indicator are water flow inputs and type of water. Best case is 0 or when no drinking water is used. Worst case 1 or when all water used is drinking water.

$$\phi_{water\ type} = \frac{m_{drinking\ H2O}^{in}}{\sum_{i=1}^N m_{H2O\ i}^{in}} \quad (26)$$

V. GREENSCOPE Environmental Indicator Evaluation Page

This data output worksheet contains the calculated environmental indicator results. In Addition, it has several columns displaying the indicators' number, name, symbol, definition, equations, absolute calculated values, units, worst and best case scenario values, and the calculated dimensionless percentage scores. Figure 16 shows a screenshot from the Efficiency page. The Environmental, Economic, and Energy Indicator Evaluation worksheet are arranged in the same format as described for the Efficiency Indicator tab.

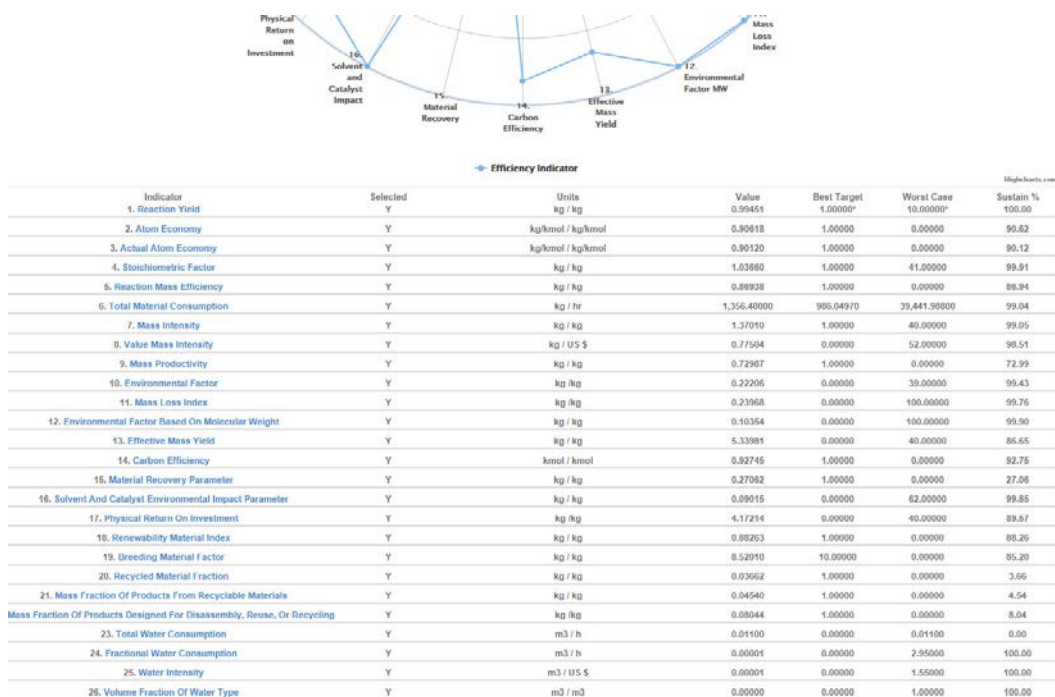


Figure 16. The Environment indicator tab shows the indicator results as well as the indicator units, worst and best case scenario values, and the dimensionless indicator results.

10. Environmental Indicators

The GREENSCOPE tool contains 66 environmental indicators. For process inputs only indicators based on hazard categorization are considered. Table 1 in Ruiz-Mercado et al. (2012)²³ provides a list of the 66 indicators used for the assessment of process sustainability in the environmental area. Some indicators use the specifications of process input material; other indicators are based on the operating conditions and process operation failures (health and safety hazards), representing the impact of components utilized in the system, and the potential impact of releases. Finally, some potential environmental impacts are quantified by the summation of potency factor contributions of different substances as equivalent amounts of a reference substance with known effect. A full explanation, mathematical formula, data needs, and worst/best case scenarios for each environmental indicator will be described below.

- 10.1. Number of hazardous materials input, $N_{\text{haz. mat.}}$. This indicator accounts for the total number of substances fed into the process, categorized as hazardous. Equation (27) represents the calculation of this indicator. The best target value is 0 or no hazardous goods and services inputs and the worst case is when all inputs are hazardous. A hazardous material list (see section 5.7.1) is necessary to obtain this indicator information.

$$N_{\text{haz. mat.}} = \sum_{i=1}^I \text{Compound}_{\text{haz. mat.}, i}^{\text{in}} \quad (27)$$

10.2. Mass of hazardous materials input, $m_{\text{haz. mat.}}$. This indicator summarizes the total amount of hazardous substances fed into the process. Equation (28) represents the calculation of this indicator. The best target and worst case values are similar to the previous indicator. In addition to a hazardous material list, process input mass flow values are required for its evaluation.

$$m_{\text{haz. mat.}} = \sum_{i=1}^I \dot{m}_{\text{haz. mat.},i}^{\text{in}} \quad (28)$$

10.3. Specific hazardous raw materials input, $m_{\text{haz. mat. spec.}}$. This indicator is the total mass of hazardous substances fed into the process per mass of valuable product. Equation (29) describes the formula used to calculate this indicator. The best target and worst case values are similar to the previous indicator, except these values are now represented per mass of valuable product. In addition to a hazardous material list and process input mass flow values, the total mass flow of valuable product(s) is required for its evaluation.

$$m_{\text{haz. mat. spec.}} = \frac{\sum_{i=1}^I \dot{m}_{\text{haz. mat.},i}^{\text{in}}}{\dot{m}_{\text{product}}} \quad (29)$$

10.4. Total mass of persistent, bio-accumulative and toxic chemicals used, $m_{\text{PBT mat.}}$. This is the total mass of substances used in the process that have persistency, bio-accumulative and toxic (PBT) properties. The formula for the calculation of this indicator is described by Equation (30). A best target is 0 or no TRI PBT inputs and worst case is when all chemicals used are identified as PBT. The TRI PBT list (see section 5.7.3) is necessary to calculate this indicator.

$$m_{\text{PBT mat.}} = \sum_{i=1}^I \dot{m}_{\text{PBT mat.},i}^{\text{in}} \quad (30)$$

10.5. Chemical Exposure Index, CEI. The Chemical Exposure Index (CEI) provides a simple method of rating the relative acute health hazard potential to people in neighboring plants or communities from possible chemical release incidents. A full description for the calculation of this indicator and its data needs is in Table 1, Ruiz-Mercado et al. (2012).¹¹ This dimensionless indicator identifies 0 as the best case scenario score and 1000 as the worst case value.

10.6. Health hazard, irritation factor, $\text{HH}_{\text{irritation}}$. This indicator assesses dermal and eye irritation to humans and animals in terms of a hypothetical volume of irritating substances in the workplace per mass of valuable product. A full description for the

calculation of this indicator and its data needs is in Table 1, Ruiz-Mercado et al. (2012).¹¹ A value of 0 m³ of irritating substances in the workplace per kg of valuable product(s) is the best case scenario and 1×10⁶ m³/kg product is the worst case scenario value.

- 10.7. Health hazard, chronic toxicity factor, $HH_{\text{chronic toxicity}}$. This is expressed as a volume of air polluted to a workplace threshold value per unit mass of valuable product. Considered aspects include: carcinogenicity, mutagenicity, reproductive toxicity, sensitization immunotoxicity, other specific (liver, lung, neural) toxicity, and odor to humans and animals. A full description for the calculation of this indicator and its data needs is in Table 1, Ruiz-Mercado et al. (2012).¹¹ A value of 0 m³ volume of air polluted to a workplace threshold value per kg of valuable product(s) is the best case scenario and 1×10⁷ m³/kg product is the worst case scenario value.
- 10.8. Safety hazard, mobility, SH_{mobility} . This indicator considers the volatility of the substances used and/or generated by the process and the capacity to generate a new gas phase in case of unexpected release of material. A value of 0.0001 kg of mass released into air in case of failure per kg of valuable product(s) is the best case scenario and 10 kg/kg product is the worst case scenario value. A set of equations (Eqns. (31) to (35)) for the calculation of this indicator is described below.

$$SH_{\text{mobility}} = \frac{m_{\text{t, air released}}^{\bullet}}{m_{\text{product}}^{\bullet}} \quad (31)$$

$$m_{\text{t, air released}}^{\bullet} = \sum_{i=1}^n PhysVal_i \times m_i^{\bullet} \quad (32)$$

$$PhysVal_i = \begin{cases} 10^{5 \times IndVal_i - 4} & \text{for } IndVal_i > 0 \\ 1 \times 10^{-4} & \text{for } IndVal_i = 0 \end{cases} \quad (33)$$

If Pv_i is known

$$IndVal_i = \begin{cases} 0.0869 \ln(Pv_i) + 0.8 & \text{if } 1 \times 10^{-4} < Pv_i < 10 \\ 1 & \text{if } Pv_i \geq 10 \\ 0 & \text{if } Pv_i \leq 1 \times 10^{-4} \end{cases} \quad (34)$$

Elseif $\Delta T_{\text{boiling}}$ is known

$$IndVal_i = \begin{cases} -0.004 \ln(\Delta T_{\text{boiling}}) + 0.8 & \text{if } 0 < \Delta T_{\text{boiling}} < 200 \\ 0.8 & \text{if } \Delta T_{\text{boiling}} \leq 0 \\ 0 & \text{if } \Delta T_{\text{boiling}} \geq 200 \end{cases} \quad (35)$$

End

The data entries for the calculation of this indicator are vapor pressure (see section 5.8.11) and standard boiling temperature (see section 5.8.11) of all process chemicals.

- 10.9. Safety hazard, fire/explosion, $SH_{\text{fire/explosion}}$. This safety hazard indicator accounts for probable energy potential releases from reaction with oxygen. The considered aspects are fuel nature, ignition source, and oxygen sources. A full description for the calculation of this indicator and its data needs is in Table 1, Ruiz-Mercado et al. (2012).¹¹ A value of 0 kJ of energy released in case of undesired fire or explosion per kg of valuable product(s) is the best case scenario and a case when all combustion enthalpy of each process substance times individual compound flow rate ($\text{maximum}[m^{\bullet\text{in}}_i, m^{\bullet\text{out}}_i]$) is released is the worst case scenario value.
- 10.10. Safety hazard, reaction / decomposition I, $SH_{\text{reac/dec I}}$. This indicator estimates the probability for undesired reaction or decomposition by considering compound thermal stability, incompatibility to air, water, acid, metal, organic substances, and exothermic reaction nature. A full description for the calculation of this indicator and its data needs is presented in Table 1, Ruiz-Mercado et al. (2012).¹¹ A zero probability for an undesired reaction or decomposition is the best case score and a probability of one is the worst case scenario score.
- 10.11. Safety hazard, reaction / decomposition II, $SH_{\text{reac/dec II}}$. This indicator estimates the amount of released energy in case undesired reactions or decomposition reactions occur during regular process operations. A set of equations (Eqns. (36) to (41)) for the calculation of this indicator is described below. There are two ways to estimate this indicator: one, by assessing the amount of energy released, and two, by accounting for an adiabatic temperature rise. The first option is the one employed in this GREENSCOPE.xls current version. A value of 0 kJ of energy released (non uncontrolled temperature rise) per kg of valuable product(s) is the best case scenario and a case when all reaction enthalpy from each process reaction is released is the worst case scenario value.

$$SH_{\text{reac/dec II}} = \frac{\sum_{i=1}^n (-\Delta H_{r,i} \times 10^{2 \times \text{IndVal}_i - 2}) \times m_i^{\bullet}}{m_{\text{product}}^{\bullet}} \text{ (Energy)} \quad (36)$$

$$SH_{\text{reac/dec II}} = \frac{\sum_{i=1}^n (-\Delta H_{r,i} \times 10^{2 \times \text{IndVal}_i - 2}) \times m_i^{\bullet}}{m_{\text{reactor}}^{\bullet\text{in}} C_{p_{\text{reactor}}}^{\text{in}}} \times \frac{1}{m_{\text{product}}^{\bullet}}} \text{ (Adiabatic temperature rise)} \quad (37)$$

$$\text{IndVal}_i = \max_i (\text{IndVal}_i) \quad (38)$$

If $-\Delta H_{\text{decomp}}$ is known

$$IndVal_i = \begin{cases} 0.0005\Delta H_{\text{decomp},i} & \text{if } 0 < -\Delta H_{\text{decomp}} < 2000 \text{ kJ/kg} \\ 1 & \text{if } -\Delta H_{\text{decomp}} \geq 2000 \text{ kJ/kg} \\ 0 & \text{if } -\Delta H_{\text{decomp}} \leq 0 \end{cases} \quad (39)$$

Elseif $-\Delta H_r$ is known

$$IndVal_i = \begin{cases} 0.0005\Delta H_{r,i} & \text{if } 0 < -\Delta H_r < 2000 \text{ kJ/kg} \\ 1 & \text{if } -\Delta H_r \geq 2000 \text{ kJ/kg} \\ 0 & \text{if } -\Delta H_r \leq 0 \end{cases} \quad (40)$$

Else NFPA-r is known

$$IndVal_i = \begin{cases} 1 & \text{if NFPA-r=3,4} \\ 0.75 & \text{if NFPA-r=2} \\ 0.25 & \text{if NFPA-r=1} \\ 0 & \text{if NFPA-r=0} \end{cases} \quad (41)$$

End

The data entries for the calculation of this indicator such as reaction enthalpy, specific thermal heat capacity, decomposition enthalpy, and NFPA-r are described in sections 5.8 and 5.7.8.

10.12. Safety hazard, acute toxicity, $SH_{\text{acute tox.}}$. This indicator assesses the potential acute toxicity from the chemical compounds by estimating a hypothetical volume of air polluted to immediate dangerous concentration per unit mass of valuable product(s). A set of equations (Eqns. (42) to (48)) needed for the calculation of this indicator is described below. A value of 0 m³ of polluted air per kg of valuable product(s) is the best case scenario and 1×10⁵ m³ per kg of product is the worst case scenario value.

$$SH_{\text{acute tox.}} = \frac{V_{\text{t, air polluted}}}{m_{\text{product}}} \quad (42)$$

$$V_{\text{t, air polluted}} = \sum_{i=1}^n PhysVal_i \times m_i \quad (43)$$

$$PhysVal_i = \begin{cases} 10^{4 \times IndVal_i + 1} & \text{for } IndVal_i > 0 \\ 0 & \text{for } IndVal_i = 0 \end{cases} \quad (44)$$

If IDLH or ERPG-3 is known

$$IndVal_i = \begin{cases} -0.109 \ln(IDLH) + 1.25 & \text{if } 10 < IDLH < 1 \times 10^5 \\ 1 & \text{if } IDLH \leq 10 \\ 0 & \text{if } IDLH \geq 1 \times 10^5 \end{cases} \quad (45)$$

Elseif EC_{class} is known

$$IndVal_i = \begin{cases} 0.875 & \text{if } EC_{class} = T^+ \\ 0.625 & \text{if } EC_{class} = T \\ 0.375 & \text{if } EC_{class} = Xn \end{cases} \quad (46)$$

Elseif GK is known

$$IndVal_i = \begin{cases} 1.0 & \text{if } GK=1 \\ 0.875 & \text{if } GK=2 \\ 0.625 & \text{if } GK=3 \\ 0.375 & \text{if } GK=4 \\ 0.125 & \text{if } GK=5 \\ 0 & \text{if } GK=\{\} \end{cases} \quad (47)$$

Elseif R_{code} is known

$$IndVal_i = \begin{cases} 0.875 & \text{if } R_{code} = 26/27/28/29, 32 \\ 0.625 & \text{if } R_{code} = 23/24/25, 31 \\ 0.375 & \text{if } R_{code} = 20/21/22 \end{cases} \quad (48)$$

End

The data needs for the calculation of this indicator such as IDLH, EC_{class} , R_{code} , and GK are described in sections 5.4 and 5.7.

10.13. Fault tree assessment, FTA. FTA is the probability of system failure if the reliability of the individual components is known. An undesired event or critical process state (safety failure) should be specified. Then, the PFD and process operating conditions are analyzed to propose and estimate different alternatives in which the undesired event can take place. A graphical model (fault tree) can be built from many consecutive or parallel combinations of faults resulting in the manifestation of the critical undesired event. Fault paths can be related to equipment failure, human errors, external events, etc. After combining these series of lower level events by using Boolean logic, a probability of the occurrence of the main safety failure event can be quantified. Indicator values are on a range between a zero probability of occurrence (best case) and a probability of one (worst case) for such main safety failure event.

10.14. Specific toxic release, TR_s . It is defined as the total mass release of toxics recognized by regulatory systems (i.e., TRI) per mass of product. Equation (49) describes the calculation of this indicator. The best case value is no releases of TRI toxics (0) and the worst case is all waste is TRI and is released without treatment.

$$TR_s = \frac{\sum_{i=1}^I m_{\text{TRI mat., } i}^{\bullet \text{out}}}{m_{\text{product}}^{\bullet}} \quad (49)$$

10.15. Toxic release intensity, TR. It is defined as the total mass release of toxics recognized by regulatory systems (i.e., TRI) per sales revenue (S_m). Liquid and gas releases are included, under each TRI category. Worst and best case values are similar to the ones for the previous indicator. Equation (50) describes the calculation of this indicator.

$$TR = \frac{\sum_{i=1}^I m_{\text{TRI mat., } i}^{\bullet \text{out}}}{S_m} \quad (50)$$

10.16. Environmental quotient, EQ. EQ is a characterization of the environmental unfriendliness of the produced waste. This is computed multiplying the E factor (Efficiency indicator #10) by the quotient Q . Q is an assigned coefficient that can be 1 if the waste is identified as innocuous, while for toxic materials such as heavy metals, Q could be a scalar between 100-1000. In the case of heterogeneous multicomponent emissions it is not possible to characterize the emissions with just one Q factor. Equations (51) and (52) describe the calculation of this indicator. Where E is the E factor material efficiency indicator. The best case value is a 0 EQ value or Q is zero for each waste component and the worst case is when all identified waste components have a Q value of 500 and are released without treatment.

$$EQ = E \times Q \quad (51)$$

$$EQ = \frac{\sum_{i=1}^I m_{\text{waste } i \neq \text{H}_2\text{O}}^{\bullet \text{out}} \times Q_i}{m_{\text{product}}^{\bullet}} \quad (52)$$

10.17. Human health burden, cancer effects, $EB_{\text{cancer eff.}}$. This indicator combines the potential factor for human health of chemical compounds in terms of their carcinogenic effects. This is accounted for as the total mass of benzene equivalents per sales revenue or value added. Equation (53) describes the calculation of this indicator. The benzene potency factor is described in section 5.10. A value of 0 or no

carcinogenic releases is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario.

$$EB_{\text{cancer eff.}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{Benzene}, i}}{S_m} \quad (53)$$

10.18. Environmental hazard, persistency of organic substances, $EH_{\text{degradation}}$. This indicator considers these aspects: Aquatic: biodegradation and hydrolysis, Air: photolysis, Soil: biodegradation. A hypothetical physical value represents the mass released of organic substances at steady state conditions per unit mass of desired product. A set of equations (Eqns. (54) to (59)) used for the calculation of this indicator is described below. OECD28d and half-life data inputs are described in section 5.5. A value of 0 kg of organic waste per kg of valuable product(s) is the best case scenario and 1 kg per kg of product is the worst case scenario value.

$$EH_{\text{degradation}} = \frac{m_{\text{t, organic}}^{\bullet}}{m_{\text{product}}^{\bullet}} \quad (54)$$

$$m_{\text{t, organic}}^{\bullet} = \sum_{i=1}^n PhysVal_i \times m_i^{\bullet} \quad (55)$$

$$PhysVal_i = \begin{cases} 10^{2 \times IndVal_i - 2} & \text{for } IndVal_i > 0 \\ 0.01 & \text{for } IndVal_i = 0 \end{cases} \quad (56)$$

$$IndVal_i = \max_i (IndVal_i) \quad (57)$$

If half-life is known

$$IndVal_i = \begin{cases} 0.2171 \ln(\text{halflife}) - 0.001 & \text{if } 1 < \text{halflife} < 100 \\ 1 & \text{if } \text{halflife} \geq 100 \\ 0 & \text{if } \text{halflife} \leq 1 \end{cases} \quad (58)$$

Elseif OECD28d (%) is known

$$IndVal_i = \begin{cases} 0.0002(\text{OECD28d})^2 - 0.0313(\text{OECD28d}) + 1.5553 & \text{if } 20 < \text{OECD28d} < 99.8 \\ 1 & \text{if } \text{OECD28d} \leq 20 \\ 0 & \text{if } \text{OECD28d} \geq 99.8 \end{cases}$$

(59)

End

10.19. Environmental hazard, air hazard, EH_{air} . This indicator accounts air hazard impacts by estimating a hypothetical volume of limit concentration air emission equivalents. Carcinogenicity, mutagenicity, reproductive toxicity, and sensitization to humans and environment are the hazard aspects that have been considered. A set of equations (Eqns. (60) to (66)) for the calculation of this indicator is described below. The data needs for the calculation of this indicator such as MAK, EC_{class} , R_{code} , and GK are described in sections 5.4 and 5.7. A value of 0 m³ volume of air polluted to a workplace threshold value per kg of valuable product(s) is the best case scenario and 1×10^7 m³/kg product is the worst case scenario value.

$$HH_{air} = \frac{V_{t, air\ polluted}}{m_{product}} \quad (60)$$

$$V_{t, air\ polluted} = \sum_{i=1}^n PhysVal_i \times m_i \quad (61)$$

$$PhysVal_i = \begin{cases} 10^{5 \times IndVal_i + 2} & \text{for } IndVal_i > 0 \\ 0 & \text{for } IndVal_i = 0 \end{cases} \quad (62)$$

If MAK-CH is known

$$IndVal_i = \begin{cases} -0.087 \ln(MAK-CH) + 0.8 & \text{if } 0.1 < MAK-CH < 1 \times 10^4 \\ 1 & \text{if } MAK-CH \leq 0.1 \\ 0 & \text{if } MAK-CH \geq 1 \times 10^4 \end{cases} \quad (63)$$

Elseif EC_{class} is known

$$IndVal_i = \begin{cases} 0.7 & \text{if } EC_{class} = T^+ \\ 0.5 & \text{if } EC_{class} = T \\ 0.3 & \text{if } EC_{class} = Xn \end{cases} \quad (64)$$

Elseif GK is known

$$IndVal_i = \begin{cases} 0.8 & \text{if } GK=1 \\ 0.7 & \text{if } GK=2 \\ 0.5 & \text{if } GK=3 \\ 0.3 & \text{if } GK=4 \\ 0.1 & \text{if } GK=5 \\ 0 & \text{if } GK=\{\} \end{cases} \quad (65)$$

Elseif R_{code} is known

$$IndVal_i = \begin{cases} 1 & \text{if } R_{code} = 45/46/47, 49, 60/61 \\ 0.8 & \text{if } R_{code} = 40, 62/63/64 \\ 0.7 & \text{if } R_{code} = 29, 32, 48 \\ 0.6 & \text{if } R_{code} = 42/43 \\ 0.5 & \text{if } R_{code} = 31, 33 \\ 0 & \text{if } R_{code} = \text{other} \end{cases} \quad (66)$$

End

10.20. Environmental hazard, water hazard, EH_{water} . This indicator evaluates the toxicity to the aquatic environment. This is a hypothetical volume of limit concentration water release equivalents per unit mass of desired product. A set of equations (Eqns. (67) to (73)) for the calculation of this indicator is described below. The data needs for the calculation of this indicator such as LC_{50} , R_{code} , and GWK are described in sections 5.6 and 5.7. A value of 0 m^3 volume of water polluted to a limit concentration release equivalents per kg of valuable product(s) is the best case scenario and 1×10^5 m^3/kg product is the worst case scenario value.

$$EH_{water} = \frac{V_{t, \text{water polluted}}}{m_{\text{product}}} \quad (67)$$

$$V_{t, \text{water polluted}} = \sum_{i=1}^n PhysVal_i \times m_i \quad (68)$$

$$PhysVal_i = \begin{cases} 10^{4 \times IndVal_i + 1} & \text{for } IndVal_i > 0 \\ 0 & \text{for } IndVal_i = 0 \end{cases} \quad (69)$$

$$IndVal_i = \max_i (IndVal_i) \quad (70)$$

If LC_{50} acute is known

$$IndVal_i = \begin{cases} -0.109 \ln(LC_{50}) + 0.75 & \text{if } 0.1 < LC_{50} < 1000 \\ 1 & \text{if } LC_{50} \leq 0.1 \\ 0 & \text{if } LC_{50} \geq 1000 \end{cases} \quad (71)$$

Elseif R_{code} is known

$$IndVal_i = \begin{cases} 0.875 & \text{if } R_{code} = 50 \\ 0.625 & \text{if } R_{code} = 51 \\ 0.375 & \text{if } R_{code} = 52 \\ 0 & \text{if } R_{code} = \text{other} \end{cases} \quad (72)$$

Elseif GWK is known

$$IndVal_i = \begin{cases} 0.875 & \text{if } GWK=3 \\ 0.5 & \text{if } GWK=2 \\ 0.125 & \text{if } GWK=1 \\ 0 & \text{if } GWK=nwg \end{cases} \quad (73)$$

End

10.21. Environmental hazard, solid waste (inorganic pollutants), EH_{solid} . This is the solid waste identified for disposal via landfill or wastewater. The total mass of inorganic dry solid waste is assessed and equation (74) describes the calculation of this indicator. A zero mass of solids per mass of valuable product(s) is the best case and 1 kg of total solids per mass of valuable product is the worst case scenario for this indicator. The categorization of solid waste is based on data provided in section 5.2.3.

$$EH_{solid} = \frac{\sum_{i=1}^N m_{inorganic\ solid\ i}^{\bullet out}}{m_{product}^{\bullet}} \quad (74)$$

10.22. Environmental hazard, bioaccumulation (in the food chain or in soil), EH_{bioacc} .

This indicator estimates the amount of mass of potential releases (including products) to accumulate in the food chain, in soil, and in inorganic matter. A set of equations (Eqns. (67) to (73)) for the calculation of this indicator is described below. The data needs for the calculation of this indicator such as BCF, R_{code} , and K_{ow} are described in sections 5.5 and 5.7.5. A value of 0 kg of inorganic solid waste per kg of valuable product(s) is the best case scenario and a 100 kg/kg product(s) is the worst case scenario value.

$$EH_{bioacc} = \frac{m_{t, acc. food\ ch.}^{\bullet}}{m_{product}^{\bullet}} \quad (75)$$

$$m_{i, \text{acc. food ch.}}^{\bullet} = \sum_{i=1}^n \text{PhysVal}_i \times m_i^{\bullet} \quad (76)$$

$$\text{PhysVal}_i = \begin{cases} 10^{2 \times \text{IndVal}_i} & \text{for } \text{IndVal}_i > 0 \\ 1 & \text{for } \text{IndVal}_i = 0 \end{cases} \quad (77)$$

$$\text{IndVal}_i = \max_i (\text{IndVal}_i) \quad (78)$$

If $\log(\text{BCF})$ is known

$$\text{IndVal}_i = \begin{cases} 0.5 \log(\text{BCF}) - 1.0 & \text{if } 2 < \log(\text{BCF}) < 4 \\ 1 & \text{if } \log(\text{BCF}) \geq 4 \\ 0 & \text{if } \log(\text{BCF}) \leq 2 \end{cases} \quad (79)$$

Elseif $\log(\text{Kow})$ is known

$$\text{IndVal}_i = \begin{cases} 0.5 \log(\text{Kow}) - 1.5 & \text{if } 3 < \log(\text{Kow}) < 5 \\ 1 & \text{if } \log(\text{Kow}) \geq 5 \\ 0 & \text{if } \log(\text{Kow}) \leq 3 \end{cases} \quad (80)$$

Elseif R_{code} is known

$$\text{IndVal}_i = \begin{cases} 1.0 & \text{if } R_{\text{code}} = 48, 53, 58 \\ 0.5 & \text{if } R_{\text{code}} = 33 \\ 0 & \text{if } R_{\text{code}} = \text{other} \end{cases} \quad (81)$$

End

10.23. Global warming potential, GWP. This is the total mass of carbon dioxide equivalents emitted per unit mass of valuable product(s). This indicator can include CO₂ equivalents (CO₂e) emitted as a byproduct, from the treatment of waste streams, and from the burning of fuel needed to generate energy for the process. The CO₂ emissions resulting from the generation of electricity and steam can be included in this indicator, even when energy utilities (electricity, steam, cooling water) are purchased rather than generated onsite. The current GREENSCOPE tool does not account for indirect CO₂e emissions unless the user includes them. Equation (82) describes the calculation of this indicator. A zero mass of CO₂e emissions per mass of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of CO₂e is based on data provided in section 5.10.

$$\text{GWP} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{CO}_2, i}}{m_{\text{product}}^{\bullet}} \quad (82)$$

10.24. Global warming potential, GWP. This is the total mass of carbon dioxide equivalents emitted per sales revenue. Equation (83) describes the calculation of this indicator. A zero mass of CO₂e emissions per sales revenue of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$\text{GWI} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{CO}_2, i}}{S_m} \quad (83)$$

10.25. Stratospheric ozone-depletion potential, ODP. The atmospheric impact measured by this indicator is based on the potential of each chemical substance to deplete ozone relative to the ODP from chlorofluorocarbon-11. This gives the total mass of CFC-11 equivalents (CFC-11e) of the process per unit mass of valuable product(s). Equation (84) describes the calculation of this indicator. A zero mass of CFC-11e emissions per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of CFC-11e is based on data provided in section 5.10.

$$\text{ODP} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{CFC-11}, i}}{m_{\text{product}}^{\bullet}} \quad (84)$$

10.26. Stratospheric ozone-depletion intensity, ODI. This gives the total mass of CFC-11 equivalents of the process per sales revenue. Equation (85) describes the calculation of this indicator.

$$\text{ODI} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{CFC-11}, i}}{S_m} \quad (85)$$

10.27. Photochemical oxidation (smog) potential, PCOP. This indicator is based on the potential of each substance to create ozone relative to the photochemical ozone creation from ethylene. This gives the total mass of ethylene equivalents (ethylene-e) of the process per unit mass of valuable product(s). Equation (84) describes the calculation of this indicator. A zero mass of ethylene-e emissions per kilogram of

valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of ethylene-e is based on data provided in section 5.10.

$$\text{PCOP} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{ethylene}, i}}{m_{\text{product}}^{\bullet}} \quad (86)$$

10.28. Photochemical oxidation (smog) intensity, PCOI. This indicator is based on the potential of each substance to create ozone relative to the photochemical ozone creation from ethylene. This gives the total mass of ethylene equivalent (ethylene-e) of the process per sales revenue of valuable product(s). Equation (87) describes the calculation of this indicator.

$$\text{PCOI} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{ethylene}, i}}{S_m} \quad (87)$$

10.29. Atmospheric acidification potential, AP. This indicator assesses the potential of chemical substances to form acid rain and acidify water. The capacity of sulphur dioxide (SO₂) to form atmospheric acidification is used as a reference unit. This gives the total mass of sulphur dioxide equivalents (SO₂e) of atmospheric acidification per unit mass of valuable product(s). Equation (88) describes the calculation of this indicator. A zero mass of SO₂e emissions per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of SO₂e is based on data provided in section 5.10.

$$\text{AP} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{SO}_2, i}}{m_{\text{product}}^{\bullet}} \quad (88)$$

10.30. Atmospheric acidification intensity, API. This gives the total mass of SO₂e of the process producing atmospheric acidification per sales revenue of valuable product(s). Equation (89) describes the calculation of this indicator. A zero mass of SO₂e emissions per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$API = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{SO_2, i}}{S_m} \quad (89)$$

10.31. Aquatic acidification potential, $WP_{\text{acid. water}}$. This aquatic impact assessment is based on the potential of chemical substances to release H^+ ions and altering the water pH. The total mass of released H^+ ions by unit mass of acid (the number of H^+ released divided by its MW) is the water acidification PF_{H^+} . The total mass of H^+ equivalents (H^+e) per mass of valuable product(s) is the unit of this environmental burden. Equation (90) describes the calculation of this indicator. A zero mass of H^+e releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of H^+e is based on data provided in section 5.10.

$$WP_{\text{acid. water}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{H^+, i}}{m_{\text{product}}^{\bullet}} \quad (90)$$

10.32. Aquatic acidification intensity, $WPI_{\text{acid. water}}$. The total mass of H^+ equivalents (H^+e) per sales revenue is the unit of this environmental burden. Equation (91) describes the calculation of this indicator. A zero mass of H^+e releases per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$WPI_{\text{acid. water}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{H^+, i}}{S_m} \quad (91)$$

10.33. Aquatic basification potential, $WP_{\text{basi. water}}$. This aquatic impact assessment is based on the potential of chemical substances to release OH^- ions and alter the water pH. The total mass of released OH^- ions by unit mass of base (the number of OH^- released divided by its MW) is the water basification, PF_{OH^-} . The total mass of OH^- equivalents (OH^-e) per mass of valuable product(s) is the unit of this environmental burden. Equation (92) describes the calculation of this indicator. A zero mass of OH^-e releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of OH^-e is based on data provided in section 5.10.

$$WP_{\text{basi. water}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{OH}^-, i}}{m_{\text{product}}^{\bullet}} \quad (92)$$

10.34. Aquatic basification intensity, $WPI_{\text{basi. water}}$. The total mass of OH^- equivalents (OH^-e) per sales revenue is the unit of this environmental burden. Equation (93) describes the calculation of this indicator. A zero mass of OH^-e releases per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$WPI_{\text{basi. water}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{OH}^-, i}}{S_m} \quad (93)$$

10.35. Aquatic salinization potential, WP_{salinity} . The aquatic impact assessment of this indicator is based on the amount of dissolved organic and inorganic salts in water. The total mass of released (Na^+ , Cl^- , K^+ , Ca^{2+} , Mg^{2+} , SO_4^{2-}), etc. salts by unit mass of base (the number of salt ions released divided by its MW) is the water salinization PF. The total mass of salt forming ions equivalents (salt-e) per mass of valuable product(s) is the unit of this environmental burden. Equation (94) describes the calculation of this indicator. A zero mass of salt-e releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of salt-e is based on data provided in section 5.10.

$$WP_{\text{salinity}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}}}{m_{\text{product}}^{\bullet}} \quad (94)$$

$$i = \text{Na}^+, \text{Cl}^-, \text{SO}_4^{2-}, \text{Mg}^{2+}, \text{Ca}^{2+}, \text{K}^+, \text{etc.}$$

10.36. Aquatic salinization intensity, WPI_{salinity} . The total mass of released (Na^+ , Cl^- , K^+ , Ca^{2+} , Mg^{2+} , SO_4^{2-}) ions per sales revenue is the unit of this environmental burden. Equation (95) describes the calculation of this indicator. A zero mass of salt-e releases per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$\text{WPI}_{\text{salinity}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}}}{S_m} \quad (95)$$

$i = \text{Na}^+, \text{Cl}^-, \text{SO}_4^{2-}, \text{Mg}^{2+}, \text{Ca}^{2+}, \text{K}^+, \text{etc.}$

10.37. Aquatic oxygen demand potential, $\text{WP}_{\text{O}_2 \text{ dem.}}$. The stoichiometric oxygen demand, StOD, represents the maximum potential of releases to water to remove dissolved O_2 that could support aquatic life. This indicator is expressed as mass of O_2 potentially removed per mass of substance per mass of valuable product(s). Equation (96) describes the calculation of this indicator. A zero mass of waste with potential to remove dissolved oxygen per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of stoichiometric oxygen demand is based on data provided in section 5.10.

$$\text{WP}_{\text{O}_2 \text{ dem.}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{O}_2 \text{ removal}, i}}{m_{\text{product}}^{\bullet}} \quad (96)$$

10.38. Aquatic oxygen demand intensity, $\text{WPI}_{\text{O}_2 \text{ dem.}}$. This indicator is expressed as mass of O_2 potentially removed per mass of substance per sales revenue. Equation (97) describes the calculation of this indicator. A zero mass of waste with potential to remove dissolved oxygen per sales revenue of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$\text{WPI}_{\text{O}_2 \text{ dem.}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times \text{PF}_{\text{O}_2 \text{ removal}, i}}{S_m} \quad (97)$$

10.39. Ecotoxicity to aquatic life potential, $\text{WP}_{\text{tox. other.}}$. This aquatic impact assessment indicator is based on the reciprocal of the Environmental Quality Standard (EQS) of the substance divided by the reciprocal of the EQS of formaldehyde, $\text{PF}_{\text{formaldehyde}}$. This indicator is expressed as mass of formaldehyde equivalents released per mass of valuable product(s). Equation (98) describes the calculation of this indicator. No formaldehyde equivalent releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The substance categorization of formaldehyde equivalents is based on data provided in section 5.10.

$$WP_{\text{tox. other}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{formaldehyde}, i}}{m_{\text{product}}^{\bullet}} \quad (98)$$

10.40. Ecotoxicity to aquatic life intensity, $WPI_{\text{tox. other}}$. This indicator is expressed as mass of formaldehyde equivalents released per sales revenue of valuable product(s). Equation (99) describes the calculation of this indicator. No formaldehyde equivalent releases per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$WPI_{\text{tox. other}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{formaldehyde}, i}}{S_m} \quad (99)$$

10.41. Ecotoxicity to aquatic life potential by metals, $WP_{\text{tox. metal}}$. This indicator is based on the reciprocal of the EQS of the chemical compounds (metals) over the reciprocal of the EQS of copper. This indicator is expressed as mass of copper equivalents released per mass of valuable product(s). Equation (100) describes the calculation of this indicator. No copper equivalent releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The substance categorization of copper equivalents is based on data provided in section 5.10.

$$WP_{\text{tox. metal}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{Cu}, i}}{m_{\text{product}}^{\bullet}} \quad (100)$$

10.42. Ecotoxicity to aquatic life potential by metals intensity, $WPI_{\text{tox. metal}}$. This indicator is expressed as mass of copper equivalents released per sales revenue from valuable product(s). Equation (101) describes the calculation of this indicator. No copper equivalent releases per sales revenue is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$WPI_{\text{tox. metal}} = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{Cu}, i}}{S_m} \quad (101)$$

10.43. Eutrophication potential, EP. The impact assessed through this indicator is defined as the potential for over-fertilization of water and soil, resulting in incremental

biomass growth in the water. The phosphate capacity to generate eutrophication is used as a reference unit. This gives the total mass of phosphate equivalents of the process releases, which cause eutrophication per unit mass of valuable product(s). Equation (102) describes the calculation of this indicator. A zero mass of phosphate equivalent releases per kilogram of valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator. The categorization of phosphate equivalent is based on data provided in section 5.10.

$$EP = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{phosphate}, i}}{m_{\text{product}}^{\bullet}} \quad (102)$$

10.44. Eutrophication potential intensity, EPI. This indicator gives the total mass of phosphate equivalents of the process releases, which create eutrophication per sales revenue. Equation (103) describes the calculation of this indicator. A zero mass of phosphate equivalent releases per sales revenue from valuable product(s) is the best case and a hypothetical scenario where any waste released has a potency factor at least equal to one is the worst case scenario for this indicator.

$$EPI = \frac{\sum_{i=1}^I m_i^{\bullet \text{out}} \times PF_{\text{phosphate}, i}}{S_m} \quad (103)$$

10.45. Specific energy intensity, SMI_M . Energy intensity describes quantitatively the amount of exergy (SeJ) consumed by ecological processes to generate the raw materials, emission dissipation, and industrial processes in order to deliver a product. Equation (104) describes the calculation of this indicator. Transformity values (Tr_i) for material flows are described in sections 5.9.1. Transformity values for energy utilities (Tr_k) have default scores in the Utility Data tab. Total product energy value per mass of product is the best case scenario and ten times the total product energy value per mass of product is the worst case scenario value for this indicator.

$$SMI_M = \frac{\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k + \sum_{i=1}^I m_i^{\bullet \text{out}} \times Tr_i}{m_{\text{product}}^{\bullet}} \quad (104)$$

10.46. Energy intensity, MI_M . This is the amount of total energy from the input and output process streams (mass and energy) divided by the sales revenue. Equation (104) describes the calculation of this indicator. Total product energy value per sales

revenue is the best case scenario and ten times the total product energy value per mass of product is the worst case scenario value for this indicator.

$$MI_M = \frac{\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k + \sum_{i=1}^I m_i^{\bullet \text{out}} \times Tr_i}{S_m} \quad (105)$$

10.47. Environmental loading ratio, ELR. This indicator is the ratio of nonrenewable net energy from purchased resources and services to renewable net energy flows. According to the literature^{24, 25}, a value of 2 is considered the best case scenario and any value higher than 10 is the worst case reference value. Equation (106) describes the calculation of this indicator. Transformity values (Tr_i) for material flows are described in sections 5.9.1 and renewability criteria are collected in sections 2.2, 4.2, and 5.2.1.

$$ELR = \frac{\left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{non-renewable}}}{\left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{renewable}}} \quad (106)$$

10.48. Energy yield ratio, EYR. This is the ratio of the energy content value from the products to the total energy consumed by the process. Equation (106) describes the calculation of this indicator. A value of 1 is considered the best case scenario and a zero value is identified as the worst case reference score.

$$EYR = \frac{m_{\text{product}}^{\bullet} \times Tr_{\text{product}}}{\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k} \quad (106)$$

10.49. Energy sustainability Index, ESI. The ESI is defined as the ratio of the EYR (indicator 48) to the ELR (indicator 47), and indicates if the process provides a suitable contribution to the user while providing a low environmental impact. This index can be used to maximize the process yield while at the lowest environmental loading (i.e. minimizing the usage of nonrenewable resources). Equation (106) describes the calculation of this indicator. According to literature^{24, 25}, a value of 5 is considered the best case scenario and a value of 1 is the worst case reference value.

$$ESI = \frac{EYR}{ELR} = \frac{\left(m_{\text{product}}^{\bullet} \times Tr_{\text{product}} \right) \left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{renewable}}}{\left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right) \left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{non-renewable}}} \quad (106)$$

10.50. Breeding factor, BF_M . This is the ratio between the total quantities of energy process outputs to the non-renewable energy content from process inputs. A value of 10 is considered the best case scenario and a zero value is assigned the worst case reference value. Equation (106) describes the calculation of this indicator.

$$BF_M = \frac{m_{\text{product}}^{\bullet} \times Tr_{\text{product}}}{\left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{non-renewable}}} \quad (106)$$

10.51. Renewability index, RI. This is the ratio of the consumption of renewable energy to the total energy supplied to the process. A value of 1 is considered the best case scenario and a zero value is the worst case reference value. Equation (106) describes the calculation of this indicator.

$$RI = \frac{\left(\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k \right)_{\text{renewable}}}{\sum_{i=1}^I m_i^{\bullet \text{in}} \times Tr_i + \sum_{k=1}^K E_k^{\bullet \text{in}} \times Tr_k} \quad (106)$$

10.52. Total solid waste mass, $m_{s, \text{tot}}$. This is representative of the total mass of solid waste produced. A value of 0 is considered the best case scenario. A worst case value of $m_{s, \text{tot}}$ is assigned with the following assumption that at least all releases having a $T_m \geq 25^{\circ}\text{C}$ or the substances that are to be land filled have potency factors equal to 1. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{tot}} = \sum_{i=1}^I m_{\text{solid}, i}^{\bullet \text{out}} \quad (106)$$

10.53. Specific solid waste mass, $m_{s, \text{spec}}$. This is the total mass of produced solid waste per unit mass of desired or valuable products. A value of 0 is considered the best case scenario. A worst case value of X is assigned with the following assumption that at least all waste having a $T_m \geq 25^{\circ}\text{C}$ or the substances that are land filled having potency factors equal to 1 are released per unit mass of desired or valuable products. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{spec.}} = \frac{\sum_{i=1}^{I'} m_{\text{solid}, i}^{\bullet \text{out}}}{m_{\text{product}}^{\bullet}} \quad (106)$$

10.54. Solid waste mass for recovery, $m_{s, \text{recov.}}$. This is the total mass of releases categorized as solid waste that can be recovered from waste streams and recycled to the process. A best case scenario value for this indicator is when all produced solid waste is recovered and 0 is the worst case scenario. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{recov.}} = \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{recoverable}} \quad (106)$$

10.55. Solid waste mass for disposal, $m_{s, \text{disp.}}$. This is the total mass of releases categorized as solid waste that cannot be recovered. A zero value is the best case scenario for this indicator and when all produced solid waste is disposed as solid waste is the worst case scenario value. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{disp.}} = \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}} \quad (106)$$

10.56. Recycling mass fraction, $w_{s, \text{recycl.}}$. This is the fraction of the total solid waste mass that is recovered for reuse in the process. A value of 1 is considered the best case scenario and a zero value is the worst case reference value. Equation (106) describes the calculation of this indicator.

$$w_{s, \text{recycl.}} = \frac{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{recoverable}}}{\sum_{i=1}^{I'} m_{\text{solid}, i}^{\bullet \text{out}}} \quad (106)$$

10.57. Disposal mass fraction, $w_{s, \text{non-recycl.}}$. This is the fraction of the total solid waste mass that cannot be recovered for reuse. A value of 0 is considered the best case scenario and a one value is the worst case reference value. Equation (106) describes the calculation of this indicator.

$$w_{s, \text{non-recycl.}} = \frac{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}}{\sum_{i=1}^{I'} m_{\text{solid}, i}^{\bullet \text{out}}} \quad (106)$$

10.58. Hazardous solid waste mass fraction, $m_{s, \text{haz}}$. This is the fraction of the total solid waste mass that cannot be recovered for reuse and is considered a hazardous waste. A value of 0 is considered the best case scenario and a value of one is the worst case reference value. Equation (106) describes the calculation of this indicator.

$$W_{s, \text{haz}} = \frac{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}^{\text{hazardous}}}{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}} \quad (106)$$

10.59. Total hazardous solid waste disposal, $m_{s, \text{haz}}$. This is the total amount of produced solid waste that cannot be recovered for reuse and is considered a hazardous waste. A value of 0 is considered the best case scenario and a worst case scenario is when all hazardous solid waste is released for disposal. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{haz}} = \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}^{\text{hazardous}} \quad (106)$$

10.60. Specific hazardous solid waste, $m_{s, \text{haz. spec}}$. This is the amount of produced hazardous waste per unit mass of valuable product. A value of 0 is considered the best case scenario and a worst case scenario is when all hazardous solid waste is released for disposal. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{haz. spec}} = \frac{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}^{\text{hazardous}}}{m_{\text{product}}^{\bullet}} \quad (106)$$

10.61. Total non-hazardous solid waste disposal, $m_{s, \text{n-haz}}$. This is the amount of produced solid waste that cannot be recovered for reuse and is considered a nonhazardous waste. When all waste is released for disposal and is categorized as nonhazardous it is considered the best case scenario and a value of 0 is the worst case scenario. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{non-haz}} = \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}} - \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}^{\text{hazardous}} \quad (106)$$

10.62. Non-hazardous solid waste intensity, $m_{s, \text{n-haz.spec}}$. This is the amount of produced solid waste that cannot be recovered for reuse and is considered a nonhazardous waste per sales revenue or value added. When all waste is released for disposal and is categorized as nonhazardous per sales revenue or value added it is considered the best

case scenario and a value of 0 is the worst case scenario. Equation (106) describes the calculation of this indicator.

$$m_{s, \text{ non-haz. spec.}} = \frac{\sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}} - \sum_{i=1}^{I'} (m_{\text{solid}, i}^{\bullet \text{out}})_{\text{non-recoverable}}^{\text{hazardous}}}{S_m} \quad (106)$$

10.63. Total volume of liquid waste, $V_{l, \text{ tot.}}$. This is the total volume of produced liquid waste. A value of 0 is considered the best case scenario and the worst case value is assuming that all waste streams (non-gas phase) are released. Equation (106) describes the calculation of this indicator. Density values (ρ) are described in section 5.8.

$$V_{l, \text{ tot.}} = \sum_{i=1}^{I'} (\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}} \quad (106)$$

10.64. Specific liquid waste volume, $V_{l, \text{ spec.}}$. This is the total volume of produced liquid waste per unit mass of desired or valuable products. A value of 0 is considered the best case scenario and the worst case value is assuming that all waste streams (non-gas phase) are released per unit mass of desired or valuable products. Equation (106) describes the calculation of this indicator. Density values (ρ) are described in section 5.8.

$$V_{l, \text{ spec.}} = \frac{\sum_{i=1}^{I'} (\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}}}{m_{\text{product}}^{\bullet}} \quad (106)$$

10.65. Non-polluted liquid waste volume, $V_{l, \text{ non-poll.}}$. This is the amount of produced liquid waste that cannot be recovered for reuse and is considered a nonhazardous waste. When all waste is discharged for disposal and is categorized as nonhazardous it is considered the best case scenario and a value of 0 is the worst case scenario. Equation (107) describes the calculation of this indicator. Density values (ρ) are described in section 5.8.

$$V_{l, \text{ non-poll.}} = \sum_{i=1}^{I'} (\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}} - \sum_{i=1}^{I'} \left((\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}} \right)_{\text{non-hazardous}} \quad (107)$$

10.66. Polluted liquid waste volume, $V_{l, \text{ poll.}}$. This is the amount of produced liquid waste that cannot be recovered for reuse and is considered a hazardous waste. When all waste is discharged for disposal and is categorized as hazardous it is considered the worst case

scenario and a value of 0 is the best case scenario. Equation (108) describes the calculation of this indicator. Density values (ρ) are described in section 5.8.

$$V_{1, \text{non-poll.}} = \sum_{i=1}^{I'} (\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}} - \sum_{i=1}^{I'} \left((\rho^{-1} m)_{\text{liquid}, i}^{\bullet \text{out}} \right)_{\text{hazardous}} \quad (108)$$

VI. GREENSCOPE Energy Indicator Evaluation Page

11. Energy Indicators

The GREENSCOPE tool contains a variety of energy indicators^{11, 23} based on thermodynamic properties used to obtain an energetic sustainability score, including energy (caloric) and exergy (available). Caloric energy balances provide the most practical and applicable methodologies used in industrial processes. However, aggregation rules (efficiency or equivalency factors) are needed to combine energy flows from different sources. Exergy balances offer the advantage to consider the irreversibility of the process (i.e., entropy generation), expressing the energy quality by quantifying the amount of useful work that can be obtained from a source of energy. In addition, the impact of their emissions can be represented in terms of exergy loss to the affected system. A full explanation, the mathematical formula, data needs, and worst/best case scenarios for each energy indicator will be described below.

- 11.1. Total energy consumption, E_{total} . For this indicator, expressed in MJ/h, all utilities provided to the system are expressed as flow rates of mass (e.g., steam) and energy and are aggregated by converting into primary fuel equivalent or caloric units. When the user needs to calculate the enthalpy value for any of these flow streams, this requires C_p , T , P , normal phase change temperatures, and composition (x_i). External data requirements consisting of the conversion factor into fuel energy for each utility stream (e.g., steam, cooling water, electricity) is needed in order to obtain the energy consumption in primary fuel equivalents. These values are predefined and can be found on the Utility Data worksheet (see section III). The total product energy value is the best case scenario and ten times the total product energy value is the worst case scenario value for this indicator. A set of equations (Eqns. (109) to (109)) for the calculation of this indicator is described below. Where E^* is the energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, in kJ/h; C_{factor} is the conversion factor to fuel energy for each respective utility; Q_k^* is the heat flow stream k , in kJ/h; W_k^* is the energy flow k for power needs, in kWh/h; $m_j^{\bullet \text{in}}$ is the total mass flow rate of the input stream j , in kg/h; $m_j^{\bullet \text{out}}$ is the total mass flow rate of the output stream j , in kg/h; ΔH_j is the mass enthalpy of the stream j in the respective

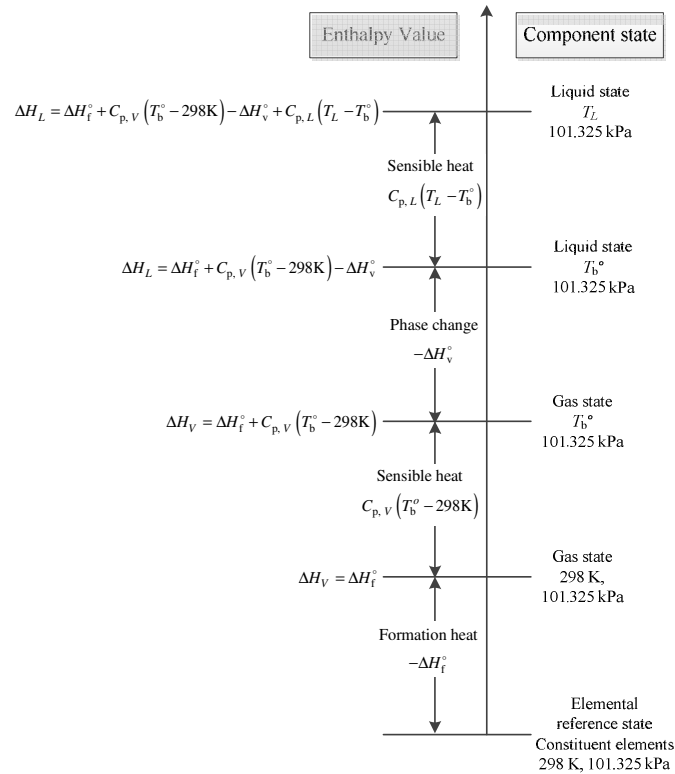
phase (L : liquid, V : vapor), in kJ/kg; $\Delta H_{j \text{ mix}}$ is the mixing enthalpy in the respective phase (L : liquid, V : vapor), in kJ/kg; and ΔH_v° is the vaporization enthalpy at standard conditions (T_0, P_0), in kJ/kg.

$$E_{\text{total}} = (C_{\text{factor}} E^\bullet)_{\text{natural gas}} + (C_{\text{factor}} E^\bullet)_{\text{fuel oil}} + (C_{\text{factor}} E^\bullet)_{\text{steam}} + \dots + (C_{\text{factor}} E^\bullet)_{\text{electricity}} \quad (109)$$

$$E^\bullet_k = \begin{cases} Q^\bullet_k & \text{heat requirements} \\ W^\bullet_k & \text{power requirements} \end{cases} \quad (109)$$

$$\sum_{j=1}^{J'} m_j^{\bullet \text{out}} \times \Delta H_j + \sum_{k=1}^K Q^\bullet_k + \sum_{k=1}^{K'} W^\bullet_k - \sum_{j=1}^J m_j^{\bullet \text{in}} \times \Delta H_j = 0 \quad (109)$$

The calculation of the enthalpy of a component is calculated taking 298 K and 101.325 kPa as the elemental reference state. A schematic representation is shown below:



$$\Delta H_{L,j} = \sum_{i=1}^c x_{i,j} \Delta H_{L,ij} + \Delta H_{L,j \text{ mix}} \quad (109)$$

$$\Delta H_{V,j} = \sum_{i=1}^c y_{i,j} \Delta H_{V,ij} + \Delta H_{V,j \text{ mix}} \quad (109)$$

11.2. Specific energy intensity, R_{SEI} . This indicator describes quantitatively the total energy consumed by the process or process operating unit in primary fuel equivalents needed to produce a product per unit mass of valuable product(s). Equation (109) describes the calculation of this indicator. Total product energy (caloric) value per mass of product is the best case scenario and ten times the total product energy value per mass of product is the worst case scenario value for this indicator.

$$R_{SEI} = \frac{(C_{\text{factor}} E^{\bullet})_{\text{natural gas}} + (C_{\text{factor}} E^{\bullet})_{\text{fuel oil}} + (C_{\text{factor}} E^{\bullet})_{\text{steam}} + \dots + (C_{\text{factor}} E^{\bullet})_{\text{electricity}}}{m_{\text{product}}^{\bullet}} \quad (109)$$

11.3. Energy intensity, R_{EI} . This is a measure of the net fuel-energy consumed to provide the heat and the power required to the process or process unit(s) per unit of sales revenue or value added. Equation (109) describes the calculation of this indicator. The total product energy (caloric) value per sales revenue is the best case scenario and ten times the total product energy value per sales revenue is the worst case scenario value for this indicator.

$$R_{EI} = \frac{(C_{\text{factor}} E^{\bullet})_{\text{natural gas}} + (C_{\text{factor}} E^{\bullet})_{\text{fuel oil}} + (C_{\text{factor}} E^{\bullet})_{\text{steam}} + \dots + (C_{\text{factor}} E^{\bullet})_{\text{electricity}}}{S_m} \quad (109)$$

11.4. Waste treatment energy, WTE. This indicator describes the net amount of energy required by the process unit(s), which are related to the processing the output waste streams per unit mass of valuable product(s). Equation (109) describes the calculation of this indicator. A zero energy (caloric) value per mass of product is the best case scenario and a ten percent (10%) of the total energy consumed per mass of product is the worst case scenario value for this indicator.

$$WTE = \frac{\left[(C_{\text{factor}} E^{\bullet})_{\text{natural gas}} + (C_{\text{factor}} E^{\bullet})_{\text{fuel oil}} + (C_{\text{factor}} E^{\bullet})_{\text{steam}} + \dots + (C_{\text{factor}} E^{\bullet})_{\text{electricity}} \right]_{\text{waste units}}}{m_{\text{product}}^{\bullet}} \quad (109)$$

11.5. Solvent recovery energy, SRE. This indicator describes the net amount of energy required by the process units, which are related to the processing of solvent recovery for reuse per unit mass of valuable product(s). Equation (109) describes the calculation of this indicator. A zero energy (caloric) value per mass of product is the best case scenario and a ten percent (10%) of the total energy consumption per mass of product is the worst case scenario value for this indicator.

$$\text{SRE} = \frac{\left[(C_{\text{factor}} E^{\bullet})_{\text{natural gas}} + (C_{\text{factor}} E^{\bullet})_{\text{fuel oil}} + (C_{\text{factor}} E^{\bullet})_{\text{steam}} + \dots + (C_{\text{factor}} E^{\bullet})_{\text{electricity}} \right]_{\text{solvent recov. units}}}{m_{\text{product}}^{\bullet}} \quad (109)$$

11.6. Resource-energy efficiency, η_E . This is a ratio between the energy content of the products to the total energy content of the feedstocks represented in the same energetic unit. This defines the quantity of the raw material energy that is remaining in the desired product. Equation (109) describes the calculation of this indicator. A value of 1 is the best case scenario and zero is the worst case scenario value for this indicator.

$$\eta_E = \frac{m_{\text{product}}^{\bullet} \times \Delta H_{\text{product}}}{\sum_{j=1}^J m_j^{\bullet \text{in}} \times \Delta H_j} \quad (109)$$

11.7. Renewability-energy index, RI_E . This is the ratio of the consumption of renewable energy to the total quantity of energy supplied to the process. A value of 1 is considered the best case scenario and a zero value is the worst case reference value. Equation (109) describes the calculation of this indicator. The needed data entries for this indicator are based on the percentage of renewability for energy-based utilities (see section 8.4).

$$\text{RI}_E = \frac{(E_{\text{total}})_{\text{renewable}}}{E_{\text{total}}} \quad (109)$$

11.8. Breeding-energy factor, BF_E . This is the ratio between the total energy process outputs over the nonrenewable energy content from process inputs. A value of 10 is considered the best case scenario and a zero value is the worst case reference value. Equation (109) describes the calculation of this indicator.

$$\text{BF}_E = \frac{m_{\text{product}}^{\bullet} \times \Delta H_{\text{product}}}{\sum_{j=1}^J m_{\text{non-renewable},j}^{\bullet \text{in}} \times \Delta H_j} \quad (109)$$

11.9. Energy for recycling, E_{recycl} . This indicator describes the net amount of energy required by the process units, which are related to the recycling of unreacted reagents or unprocessed feedstocks per unit mass of valuable product(s). Equation (109) describes the calculation of this indicator. A zero energy (caloric) value per mass of product is the best case scenario and ten percent (10%) of the total energy consumption per mass of product is the worst case scenario value for this indicator.

$$E_{\text{recycl.}} = \frac{\left[\begin{array}{l} (C_{\text{factor}} E^{\bullet})_{\text{natural gas}} + (C_{\text{factor}} E^{\bullet})_{\text{fuel oil}} + (C_{\text{factor}} E^{\bullet})_{\text{steam}} \\ + \dots + (C_{\text{factor}} E^{\bullet})_{\text{electricity}} \end{array} \right]_{\text{Recycling units}}}{m_{\text{product}}^{\bullet}} \quad (109)$$

11.10. Exergy consumption, Ex_{total} . This indicator accounts for the portion of heat energy available from a stream that can be converted into useful work and the amount of useful work that can be obtained from a source of energy (heat and power). The computation of Ex for a process material stream requires the selection of reference states for the physical exergy (which accounts for differences in P and T), chemical exergy (accounting for differences in compositions with the environment at T_0 and P_0), and mixing exergy (accounting for differences with the pure state of the mixture components). The same reference state used as for caloric energy ($T_0 = 298.15$ K and $P_0 = 101.325$ kPa) is assumed here, with the addition of the environmental reference state for the chemical exergy as being derived by the mean composition of the air, oceans, and a selected thickness of the earth's crust. The exergy of work is the same as the energetic value, and the exergy of a heat stream is calculated by multiplying its caloric energy value with its Carnot efficiency. A set of equations (Eqns. (109) to (109)) for the calculation of this indicator is described below. This is constituted by aggregation of the exergy of the material streams, exergy of work, and the exergy of heat streams. Therefore, data from all process streams such as H , S , x_i , Q^{\bullet} , W^{\bullet} , standard chemical exergy of substance i , (Ex_i^{och}), as well as T and P have to be known or estimated. The total product exergy value is the worst case scenario and zero exergy consumption is the best case scenario value for this indicator.

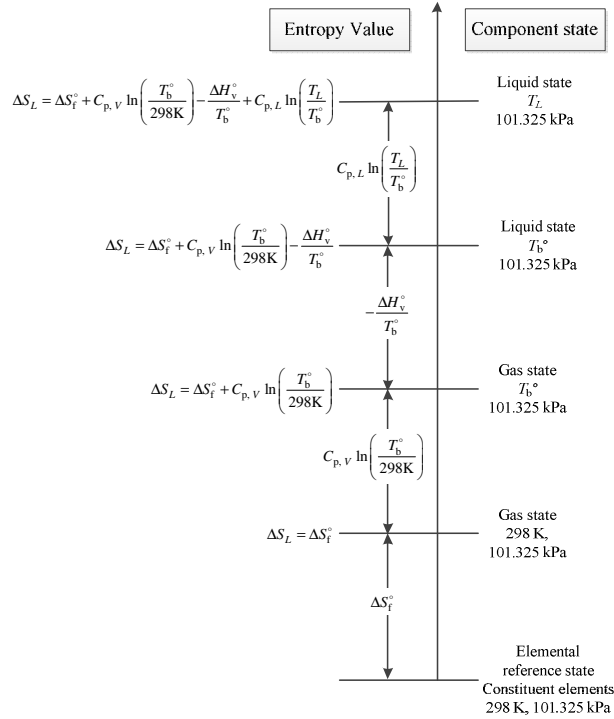
$$Ex_{\text{total}} = Ex^{\bullet \text{in}} - Ex_{\text{product}}^{\bullet} \quad (109)$$

$$Ex^{\bullet \text{in}} = [Ex^{\bullet}(\text{physical}) + Ex^{\bullet}(\text{chemical})]_{\text{input flows}} + Ex^{\bullet}(\text{work}) + Ex^{\bullet}(\text{heat}) \quad (109)$$

$$Ex^{\bullet \text{in}} = \sum_{j=1}^J m_j^{\bullet \text{in}} (\Delta H - T_0 \Delta S)_j + \sum_{j=1}^J \left[\sum_{i=1}^c n_i^{\bullet} \sum_{i=1}^c (x_i Ex_i^{\text{och}} + RT_0 x_i \ln(x_i)) \right]_j + \sum_{k=1}^{K'} W_k^{\bullet} + \sum_{k=1}^K Q_k^{\bullet} (1 - T_0 / T_{*,k}) \quad (109)$$

$$Ex_{\text{product}}^{\bullet} = m_{\text{product}}^{\bullet} (\Delta H - T_0 \Delta S)_{\text{product}} + n_{\text{product}}^{\bullet} Ex_{\text{product}}^{\text{och}} \quad (109)$$

The calculation of the entropy of a component is calculated taking 298 K and 101.325 kPa as the elemental reference state. A schematic representation is shown below:



$$\Delta S_{L,j} = \sum_{i=1}^c x_{i,j} \Delta S_{L,ij} + \Delta S_{L,j \text{ mix}} \quad (109)$$

$$\Delta S_{V,j} = \sum_{i=1}^c y_{i,j} \Delta S_{V,ij} + \Delta S_{V,j \text{ mix}} \quad (109)$$

Where $Ex^{\circ \text{in}}$ is the total exergy flow input to the process or process unit, in kJ/h; m_j° is the total mass flow rate of the stream j , in kg/h; ΔH_j is the mass enthalpy of the stream j , in kJ/kg; T_0 is the temperature of reference, $T_0=298$ K; ΔS_j is the mass entropy of the stream j , in kJ/(kg K); n_i° is the molar flow rate of substance i , in kmol/h; $Ex_i^{\circ \text{ch}}$ is the standard chemical exergy of substance i , in kJ/kmol; R is the universal gas constant, $R=8.314$ kJ/(kmol K); x_i is the molar fraction of species i ; W_k° is the energy flow k for power needs, in kWh/h; Q_k° is the heat flow stream k , in kJ/h; T_{*k} is the temperature at which a heat flow stream k is supplied, in K; $S_{\text{generated}}^{\circ}$ is the generated entropy due to the irreversibility of the system, in kJ/(h K); and ΔS_i° is the formation entropy at standard conditions (T_0, P_0), in kJ/(kg K).

11.11. Exergy intensity, R_{Ex} . This energy indicator describes quantitatively the amount of resources in exergy units needed to deliver the product per unit mass of valuable product. Equations (109) to (109) describe the calculation of this indicator. Total product exergy (caloric) value per mass of product is the best case scenario and five times the

total product exergy value per mass of product is the worst case scenario for this indicator.

$$R_{\text{Ex}} = \frac{\text{Ex}_{\text{product}}^{\bullet} - \text{Ex}_{\text{lost}}^{\bullet}}{m_{\text{product}}^{\bullet}} \quad (109)$$

$$\text{Ex}_{\text{lost}}^{\bullet} = T_0 S_{\text{generated}}^{\bullet} \quad (109)$$

$$S_{\text{generated}}^{\bullet} = \sum_{j=1}^{J'} m_j^{\bullet \text{out}} \times \Delta S_j - \sum_{j=1}^J m_j^{\bullet \text{in}} \times \Delta S_j - \sum_{k=1}^K \frac{Q_k^{\bullet}}{T_k} \quad (109)$$

11.12. Resource-exergy efficiency, η_{Ex} . This is a ratio between the exergy content of the products to the total exergy content from the process inputs. This quantifies the quantity of process exergy inputs remaining in the desired product. Equation (109) describes the calculation of this indicator. A value of one is the best case scenario and a zero value is the worst case scenario for this indicator.

$$\eta_{\text{Ex}} = \frac{\text{Ex}_{\text{product}}^{\bullet}}{\text{Ex}_{\text{in}}^{\bullet}} \quad (109)$$

11.13. Renewability-exergy index, RI_{Ex} . This is the ratio of consumption of renewable exergy to the total exergy supplied to the process. A value of 1 is considered the best case scenario and a zero value is the worst case reference value. Equation (109) describes the calculation of this indicator. The data entries for this indicator are based on the percentage of renewability for energy based utilities (see section 8.4) and feedstocks.

$$\text{RI}_{\text{Ex}} = \frac{\text{Ex}_{\text{renewable}}^{\bullet \text{in}}}{\text{Ex}_{\text{in}}^{\bullet}} \quad (109)$$

11.14. Breeding-exergy factor, BF_{Ex} . This is the ratio between the total exergy process outputs to the nonrenewable exergy content from process inputs. A value of 10 is considered the best case scenario and a zero value is the worst case reference value. Equation (109) describes the calculation of this indicator.

$$\text{BF}_{\text{Ex}} = \frac{\text{Ex}_{\text{product}}^{\bullet}}{\text{Ex}_{\text{nonrenewable}}^{\bullet \text{in}}} \quad (109)$$

VII. GREENSCOPE Economic Indicator Evaluation Page

12. Economic Indicators

The GREENSCOPE tool includes economic indicators for the assessment of process sustainability in terms of profit and costs. Indicators based on profitability criteria for projects (process, operating unit, equipment) may or may not account for the time value of money (i.e., discounted or non-discounted values). For evaluating large-scale projects, discounted techniques are recommended; however, for smaller projects (process improvements such as equipment replacement) non-discounted profitability techniques are still used. Indicators supported in cost criteria can be grouped as processing costs (e.g., capital cost, manufacturing cost), process input costs (raw material cost, utility costs), and process output costs (waste treatment costs). Different project alternatives can be compared by employing the discount rate (or interest rate, r_d) used to move all cash flows back to the beginning of the project, the time required to recover the initial investment (DPBP), and the minimum rate at which the initial investment is recovered (minimum acceptable rate of return, MARR). Combined aspects of these parameters (see section 7) are used to propose reference states for economic sustainability indicators. When $r_d=0$, it gives the best target scenario because this means that future profits maintain their value back to time zero, and it generates the shortest DPBP. The MARR has different values according to the level of risk for the investment: for a low risk project MARR is 4%/yr, and for a very high risk investment MARR is 48%/yr. More details regarding the economic indicators are described¹ in Ruiz-Mercado et al.^{1, 11, 23}

12.1. Net present value, NPV. The implementation of this profitability evaluation indicator requires process equipment are sized based on physical models. It can provide a better measurement in the evaluation of different design proposals. NPV is computed by adding the present values of all incomes (cash flows) subtracted by the summation of the present values of all capital investments. In addition, capital and manufacturing costs must be estimated before the NPV is calculated. Equations (109) to (109) describe implicit relationships between process information used as data input to calculate the above mentioned costs, which are intermediate values for assessing NPV. Where n : life of the plant or equipment, yr; $PWF_{cf,m}$: the selected present worth factor (from Table 7-3, 7-4, or 7-5 in Peters et. al.¹⁹); S_m : total income from all sales in year m , \$; COM_m : cost of manufacture without depreciation, \$; FCI_L : fixed capital investment without including the land value; d_m : depreciation charge. Here, it is assumed as 10% of the FCI_L evaluated in year m , however it can be estimated by different methods¹⁹; Φ : fixed income tax rate given by the IRS (Table 9.3 in Turton et. al. ¹⁷); rec_m : salvage-value recovered from the working capital, land value, and the sale of physical assets evaluated at the end of the

plant life. Often this salvage value is neglected, \$; b : the year in which the first investment is made before the startup time, which is represented as time zero; $PWF_{v,m}$: the appropriate present worth factor for investments occurring in year m (from Table 7-3, 7-4, or 7-5 in Peters et. al.¹⁷); TCl_m : the total capital investment in year m ; $m_{m, \text{product } i}^{\bullet}$: annual mass flow of product i in year m , kg/yr; $C_{m,i}$: cost of material¹⁹ i in year m , \$/kg; C_{UT} : cost of utilities, \$; C_{WT} : cost of waste treatment, \$; C_{RM} : cost of raw material, \$; $C_{Land,m}$: value of the land evaluated in year m , \$; WC : working capital, typical values for the WC are between 15% and 20% of the FCI_L ; C_{OL} : labor cost, \$; $C_{p,i}^o$: the purchased cost for equipment i , \$; $F_{BM,i}$: the bare module cost²⁶ of equipment i , \$; C_{TM} : the capital cost (total module) of the plant, \$; u : the total number of individual units; N_{OL} : the number of operators per shift; and P : the number of processing steps involving the handling of particulate solids (e.g., transportation and distribution). In general, $P=0$. Nnp : the number of non-particulate processing steps, including compression, heating and cooling, mixing, and reaction. A NPV calculated by employing an $r_d = 0\%$ is the best case scenario and a NPV calculated by assuming an $r_d = 40\%$ is the worst case scenario value for this indicator.

$$NPV = \sum_{m=1}^n PWF_{cf,m} [(S_m - COM_m - d_m)(1 - \Phi) + rec_m + d_m] - \sum_{m=-b}^n PWF_{v,m} TCl_m \quad (109)$$

$$S_m = \sum_{i=1}^I m_{m, \text{product } i}^{\bullet} \times C_{m, \text{product } i} \quad (109)$$

$$COM_m = 0.280FCI_{L,m} + 2.73C_{OL,m} + 1.23(C_{UT,m} + C_{WT,m} + C_{RM,m}) \quad (109)$$

$$d_m = 0.1FCI_L \quad (109)$$

$$rec_m = \begin{cases} C_{Land} + WC + FCI_L - \sum_{m=1}^n d_m & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases} \quad (109)$$

$$TCl_m = C_{Land,m} + FCI_{L,m} + WC_m \quad (109)$$

$$FCI_L = C_{TM} = 1.18 \sum_{i=1}^u C_{BM,i} \quad (109)$$

$$C_{BM,i} = C_{p,i}^o F_{BM,i} \quad (109)$$

$$C_{OL} = 4.5N_{OL} \times (\text{annual salary}) \quad (109)$$

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (109)$$

$$N_{np} = \sum \text{Equipment} \quad (109)$$

12.2. Present value ratio, PVR. This indicator is another criterion to compare different projects, which have different investment levels. Conventionally, a project describing a PVR equal to one means a break-even scenario. In addition, when $PVR > 1$, the project is profitable, and when $PVR < 1$ this represents an unprofitable design. A value of 1 is considered the worst case scenario and a PVR calculated by employing an $r_d = 0\%$ is the best case scenario. Equation (109) describes the calculation of this indicator.

$$PVR = \frac{\sum \text{positive} \left(PWF_{cf,m} \left[(S_m - COM_m - d_m)(1 - \Phi) + rec_m + d_m \right] - PWF_{v,m} TCI_m \right)}{\sum \text{negative} \left(PWF_{cf,m} \left[(S_m - COM_m - d_m)(1 - \Phi) + rec_m + d_m \right] - PWF_{v,m} TCI_m \right)} \quad (109)$$

12.3. Discounted payback period, DPBP. This indicator assesses the time required, after startup, to recover the fixed capital investment, required for the project, with all cash flows discounted back to time zero. A value of 1 year is considered the best case scenario and a value equal to the life of the plant after startup (11 yrs) is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\begin{aligned} DPBP &= n' \\ f(n') &= \sum_{m=1}^{n'} PWF_{cf,m} \left[(S_m - COM_m - d_m)(1 - \Phi) + rec_m + d_m \right] \\ &\quad - \sum_{m=-b}^{n'} PWF_{v,m} TCI_m + PWF_{v,n'} (C_{Land} + WC) = 0 \end{aligned} \quad (109)$$

12.4. Discounted cash flow rate of return, DCFROR. This indicator shows the highest, after-tax interest or discount rate at which the project can just break even. In addition, this is the r_d at which $NPV = 0$ is equal to zero and is calculated by solving equation (109). This equation is solved by using a nonlinear equation solver applied on $NPV=0$ equation. The user must run the nonlinear equation solver every time after changes to the variables or parameters affecting this indicator. This indicator so called internal rate interest is usually determined by corporate management and represents the minimum acceptable rate of return the company will accept for any new investment. A project that yields $DCFROR > d$ is considered to be profitable. A fraction of 0.4 is considered the

best case scenario and a zero value is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\begin{aligned} \text{DCFRROR} &= i \\ f(i) &= \sum_{m=1}^{n'} \text{PWF}_{\text{cf},m} \left[(S_m - \text{COM}_m - d_m)(1 - \Phi) + \text{rec}_m + d_m \right] \\ &\quad - \sum_{m=-b}^{n'} \text{PWF}_{\text{v},m} \text{TCI}_m = 0 \end{aligned} \quad (109)$$

12.5. Capital charge factors, CCF. The CCF accounts the time value of money in a profitability analysis during a preliminary process design. There is a direct relationship between CCF and the DCFRROR. The CCF is calculated by subtracting the COM to the sales revenues and normalized by the TCI. A value of $\text{CCF}=1 \text{ yr}^{-1}$ (i.e., assumed for a high risk projects) is the best case scenario and a zero value is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{CCF}_{\text{average}} = \frac{1}{n'} \sum_{m=1}^{n'} \frac{\text{PWF}_{\text{cf},m} (S_m - \text{COM}_m)}{\text{TCI}} \quad (109)$$

12.6. (Specific) Economic potential, EP. The EP indicator can be a good approximated cost model that fits into the hierarchical conceptual process design stages, mainly, when the input/output structure of the flowsheet is accounted (product sales revenue, feedstock costs, utility costs). The calculation shown here is set for the evaluation at the end of the first year when the plant is operating (second year). A value of 1 is the best-case scenario and a zero value is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{EP}_m = \frac{\text{PWF}_{\text{cf},m} (S_m - C_{\text{RM},m} - C_{\text{UT},m}) - \text{FCI}_{\text{L},m}}{\sum_{i=1}^I m_{m, \text{product } i}} \quad (109)$$

12.7. Rate of return on investment, ROI. The ROI does not consider the time value of money. It represents the non-discontinued rate at which money is earned from the FCI. The annual net profit is an average over the life of the plant after startup. If the plant salvage value (rec) is non-negligible, this value should be subtracted from FCI_{L} . A fraction value of 0.4 is the best case scenario and a zero value is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{ROI} = \frac{\frac{1}{n} \sum_{m=1}^{n'} [(S_m - \text{COM}_m - d_m)(1 - \Phi) + d_m]}{\text{FCI}_L} \quad (109)$$

12.8. Payback period, PBP. This is the time required, after startup to recover the fixed capital invested, FCI, for the project. A more profitable project has a shorter payback period. The FCI and the annual cash flow are needed to compute the PBP. Note this indicator does not consider the time value of money. A value of 1 year is considered the best case scenario and a value equal to the life of the plant after startup (11 yrs) is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{PBP} = n^* \\ f(n^*) = \sum_{m=1}^{n^*} [(S_m - \text{COM}_m - d_m)(1 - \Phi) + \text{rec}_m + d_m] - \sum_{m=-b}^{n^*} \text{FCI}_m = 0 \quad (109)$$

12.9. Turnover ratio, TR. This indicator is a faster profitability evaluation method suitable for early stages of conceptual process design. This is the ratio of gross annual sales to fixed capital investment. A value of 4 (for some business establishments) is considered the best case scenario and a ratio equal to 0.2 is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{TR} = \frac{\sum_{i=1}^I m_{m, \text{product } i} \times C_{m, \text{product } i}}{\text{FCI}_L} \quad (109)$$

12.10. Cumulative cash position, CCP. This indicator is the value of the project at the end of its assumed life. A value equal to the project's FCI_L is considered the best case scenario and a zero value is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$\text{CCP} = \sum_{m=1}^n [(S_m - \text{COM}_m - d_m)(1 - \Phi) + \text{rec}_m + d_m] - \sum_{m=-b}^n \text{TCl}_m \quad (109)$$

12.11. Cumulative cash ratio, CCR. This is a useful indicator when several projects with different FCI_L have to be compared. By definition, this is the CCP indicator normalized by the initial investment. The best case scenario value is calculated by performing a non-discontinued after tax cash flow analysis with a COM = 0.38*TPC and a TCI = 0.60*FCI. The worst case scenario value is obtained with a COM = 1.7*TPC and a TCI = 1.25*FCI. Equation (109) describes the calculation of this indicator.

$$CCR = \frac{\sum \text{positive} \left(\left[(S_m - COM_m - d_m)(1 - \Phi) + \text{rec}_m + d_m \right] - TCI_m \right)}{\sum \text{negative} \left(\left[(S_m - COM_m - d_m)(1 - \Phi) + \text{rec}_m + d_m \right] - TCI_m \right)} \quad (109)$$

12.12. Net return, R_n . This non-discounted profitability criterion is the required amount of cash flow over and above to meet the MARR and recover the total capital investment. The best case scenario value is when R_n is calculated by performing a non-discontinued after tax cash flow analysis with a $COM = 0.38*TPC$, $MARR = 0.16$, and a $TCI = 0.60*FCI$. The worst case scenario value is zero. Equation (109) describes the calculation of this indicator.

$$R_n = \sum_{m=1}^n \left[(S_m - COM_m - d_m)(1 - \Phi) \right] - MARR \left(n \sum_{m=-b}^n TCI_m \right) \quad (109)$$

12.13. Revenues from eco-products, REV. This indicator assesses the net revenues from the sale of products categorized as eco-products. A hypothetical case when all valuable products are categorized as eco-products is the best case scenario. An opposite case is when no eco-products are part of the valuable products. Equation (109) describes the calculation of this indicator.

$$REV_m = \sum_{i=1}^I m_{m, \text{eco-product } i} \times C_{m, \text{eco-product } i} \quad (109)$$

12.14. Revenue fraction of eco-products, $REV_{\text{eco-prod.}}$. This is the net revenues from the sale of products categorized as eco-products over the total sales revenue or value added. A value of 1 (all sales revenue from eco-products) is considered the best case scenario and zero is the worst case scenario. Equation (109) describes the calculation of this indicator.

$$REV_{\text{eco-prod.}} = \frac{\sum_{i=1}^I m_{m, \text{eco-product } i} \times C_{m, \text{eco-product } i}}{S_m} \quad (109)$$

12.15. Equivalent annual cost, C_{eq} . This is the sum of the annualized investment cost (AIC) calculated with a specified discount rate and the total annual outcomes after taxes. AIC is the annuity required for the TCI to be returned over the project lifetime. The total annual outcomes are the negative cash flow values. The best case scenario value is a C_{eq} calculated with a $COM = 0.38*TPC$ and a $TCI = 0.60*FCI$. The worst case scenario value is a C_{eq} obtained with a $COM = 1.7*TPC$ and a $TCI = 1.25*FCI$. Equation (109) describes the calculation of this indicator.

$$C_{eq} = \text{COM}_m + \text{PWF}_{v,m} \text{TCI}_m$$

$$\text{PWF}_{v,m} = \frac{i(1+i)^n}{(1+i)^n - 1} \quad (109)$$

12.16. Total product cost, TPC. This indicator combines the operating costs of the plant, distribution and selling the products, administrative costs, and research and development costs. The process general expenses (GE) are equal to the sum of administrative costs, distribution and selling costs, and research and development costs. According to industry reports, this value is in the range of 15% to 25% of the TPC (Peters et al. 2003 pp 259-274).¹⁹ The best case scenario value is when $\text{TPC} = 1.4 * \text{COM}_{\text{best-case}}$ and the worst case scenario value is when $\text{TPC} = 1.2 * \text{COM}_{\text{worst-case}}$. Equation (109) describes the calculation of this indicator.

$$\text{TPC} = \text{COM} + \text{GE} \quad (109)$$

12.17. Production cost, E_{pc} . Production cost can be an easy indicator to calculate if the process equipment are not sized, however all mass and energy balances are fully specified. The best case scenario value is an E_{pc} calculated with a $C_{RM} = 0.1 * \text{TPC}_{\text{best-case}}$, $C_{WT} = 0.05 * \text{TPC}_{\text{best-case}}$, and a $C_{OL} = 0.05 * \text{TPC}_{\text{best-case}}$. The worst case scenario value is an E_{pc} calculated with a $C_{RM} = 0.8 * \text{TPC}_{\text{worst-case}}$, $C_{WT} = 0.4 * \text{TPC}_{\text{worst-case}}$, and a $C_{OL} = 0.4 * \text{TPC}_{\text{worst-case}}$. Equation (109) describes the calculation of this indicator.

$$E_{PC} = \sum_{i=1}^I m_{m,i}^{\text{in}} \times C_{m,i} + \sum_{\substack{j=1 \\ j \neq \text{prod. st.}}}^{J'} C_{WT,j} m_j^{\text{out}} + C_{OL} \quad (109)$$

12.18. Capital cost, C_{TM} . Capital cost assesses the total amount of money that it takes to build a new plant or modifications to an existing chemical plant. Note that capital cost estimation at conceptual design phases would be underestimated by not including all of the equipment required in the process. A capital cost estimate along all levels of process design becomes more realistic and accurate as more detailed information (additional equipment is covered) is available. However, an economic analysis for an existing process should not be difficult since cost and profitability studies were performed prior to its construction. The best-case scenario value is calculated by performing a non-discontinued after tax cash flow analysis with a Purchase equipment cost = $0.15 * \text{FCI}$ and a $\text{TCl} = 0.60 * \text{FCI}$. The worst case scenario value is obtained when Purchase equipment cost = $0.4 * \text{FCI}$ and $\text{TCl} = 1.25 * \text{FCI}$. Equations (109), (109), (109) - (109) describe the calculation of this indicator. Where C_p° : purchased cost of equipment at manufacture's

site, \$; C_M : cost of materials required for equipment installation, \$; C_L : cost of labor to install equipment and material, \$; C_{FIT} : cost of freight, insurance, and taxes, \$; C_O : construction overhead, \$; C_E : contractor engineering expenses, \$; C_{Cont} : contingency factor, \$; and C_{Fee} : contractor fee, \$.

$$C_{TM} = \sum_{i=1}^u (C_{direct,i} + C_{indirect,i} + C_{Cont.,i} + C_{Fee,i}) \quad (109)$$

$$C_{direct} = C_p + C_M + C_L \quad (109)$$

$$C_{indirect} = C_{FIT} + C_O + C_E \quad (109)$$

12.19. Manufacturing cost, COM. These are the costs related with the day-to-day operation of a manufacturing plant. This cost must be estimated in order to assess the economic feasibility of a proposed process design. COM is constituted by direct manufacturing costs (e.g., C_{RM} , C_{WT}), fixed costs (e.g., depreciation), and general expenses (e.g., administration costs). A full list of factors affecting COM is described in Table 8.1 in Turton et al. (2009). The best case scenario value is when $COM = 0.38*TPC$ and $TCI = 0.60*FCI$. The worst case scenario value is when $COM = 1.7*TPC$ and a $TCI = 1.25*FCI$. Equations (109), (109) - (109) describe the calculation of this indicator. Where $Utility_u$: charges for utilities delivered to the battery limit of the process, \$/utility flow rate; see data inputs for NPV indicator.

$$C_{UT} = \sum_{u=1}^U (C_{UT,u} \times utility_u) \quad (109)$$

$$C_{WT} = \sum_{\substack{j=1 \\ j \neq \text{prod. st.}}}^{J'} (C_{WT,j} \times m_j^{\text{out}}) \quad (109)$$

$$C_{RM,m} = \sum_{i=1}^I (m_{m,i}^{\text{in}} \times C_{m,i}) \quad (109)$$

12.20. Specific raw material cost, C_{SRM} . C_{SRM} can be used as economic indicator at the basic conceptual process design stage, assuming 100% reaction yield, thus the minimum raw material cost is computed. Some process design routes can be discarded when C_{SRM} exceeds the targeted product value. Equation (109) describes the calculation of this indicator. The best case scenario value is when $C_{SRM} = 0.1*TPC_{\text{best-case}}$ and a worst case scenario value is when $C_{SRM} = 0.8*TPC_{\text{worst-case}}$ per unit of kilogram of valuable product(s).

$$C_{\text{SRM},m} = \frac{\sum_{i=1}^{I'} (m_{m,i}^{\bullet \text{in}} \times C_{m,i})}{\sum_{i=1}^I m_{m, \text{product } i}^{\bullet}} \quad (109)$$

12.21. Total material cost, $C_{\text{RM},m,\text{tot}}$. This is the absolute cost of total material used in the process or process unit. Equation (109) describes the calculation of this indicator. The best case scenario value is when $C_{\text{SRM}} = 0.1 * \text{TPC}_{\text{best-case}}$ and a worst case scenario value is when $C_{\text{SRM}} = 0.8 * \text{TPC}_{\text{worst-case}}$.

$$C_{\text{mat,tot}} = \sum_{i=1}^I (m_{m,i}^{\bullet \text{in}} \times C_{m,i}) \quad (109)$$

12.22. Total energy cost, $C_{\text{E,tot}}$. This is the manufacturing cost related to the utility energy demand costs during the day-to-day operation of a manufacturing plant: fuels, electricity, steam, etc. Equation (109) describes the calculation of this indicator. The best case scenario value is when only consumed energy is from the cheapest source (assumed to be coal) @ $\$1.72 \times 10^{-6}/\text{kJ}$ and a worst case scenario value is when only consumed energy is from the most expensive source (assumed to be electricity) @ $\$1.68 \times 10^{-5}/\text{kJ}$.

$$C_{\text{E,tot}} = \sum_{u=1}^{U'} (C_{\text{UT},u} \times \text{utility}_{\text{energy},u}^{\bullet}) \quad (109)$$

12.23. Average cost of energy source, $C_{\text{E,source}}$. This is the average cost related with the utility energy demand costs during the day-to-day operation of a manufacturing plant per unit of consumed energy as equivalent primary energy source. Equation (109) describes the calculation of this indicator. The best case scenario value is when $C_{\text{E,source}}$ is equal to the cost from the cheapest source (assumed to be coal) @ $\$1.72 \times 10^{-6}/\text{kJ}$ and a worst case scenario value is when $C_{\text{E,source}}$ is equal to the cost from the most expensive source (assumed to be electricity) @ $\$1.68 \times 10^{-5}/\text{kJ}$.

$$C_{\text{E,source}} = \frac{\sum_{u=1}^{U'} (C_{\text{UT},u} \times \text{utility}_{\text{energy},u}^{\bullet})}{E_{\text{total}}} \quad (109)$$

12.24. Specific energy cost, $C_{\text{E,spec}}$. These are the costs related to the utility energy demand costs during the day-to-day operation of a manufacturing plant per unit value of total production cost. Equation (109) describes the calculation of this indicator. The best case scenario value is when only consumed energy is from the cheapest source

(assumed to be coal) @ $\$1.72 \times 10^{-6}$ /kJ divided by $TPC_{\text{best-case}}$ and a worst case scenario value is when only consumed energy is from the expensive source (assumed to be electricity) @ $\$1.68 \times 10^{-5}$ /kJ divided by $TPC_{\text{worst-case}}$.

$$C_{E, \text{spec.}} = \frac{\sum_{u=1}^{U'} (C_{UT,u} \times \text{utility}_{\text{energy}, u})}{TPC} \quad (109)$$

12.25. Total water cost, $C_{\text{water tot.}}$. These are the costs related with the water demand costs during the day-to-day operation of a manufacturing plant: drinking water, process use water, boiler feed water, deionized water, etc. Equation (109) describes the calculation of this indicator. The best case scenario value is when only consumed water is from the cheapest source (assumed to be process use water) @ $\$0.067$ $\$/\text{m}^3$ and a worst case scenario value is when only consumed water is from the most expensive source (assumed to be deionized water) @ $\$1.0$ $\$/\text{m}^3$.

$$C_{\text{water tot.}} = \sum_{i=1}^w (m_{\text{H}_2\text{O},i}^{\text{in}} \times C_{\text{H}_2\text{O},i}) \quad (109)$$

12.26. Water cost fraction, $C_{\text{water spec.}}$. These are the water demand costs during the operation of a manufacturing plant normalized by the total production cost. Equation (109) describes the calculation of this indicator. The best case scenario value is when only consumed water is from the cheapest source (assumed to be process use water) @ $\$0.067$ $\$/\text{m}^3$ divided by $TPC_{\text{best-case}}$ and a worst case scenario value is when only consumed water is from the most expensive source (assumed to be deionized water) @ $\$1.0$ $\$/\text{m}^3$ divided by $TPC_{\text{worst-case}}$.

$$C_{\text{water spec.}} = \frac{\sum_{i=1}^w (m_{\text{H}_2\text{O},i}^{\text{in}} \times C_{\text{H}_2\text{O},i})}{TPC} \quad (109)$$

12.27. Average volume water type cost, $C_{\text{water type}}$. These are the costs related to the water demand costs during the day-to-day operation of a manufacturing plant per volume of total consumed water. Equation (109) describes the calculation of this indicator. The best case scenario value is a $C_{\text{water type}}$ equal to the cheapest water source (assumed to be process use water), $\$0.067$ $\$/\text{m}^3$. A worst case scenario value is a $C_{\text{water type}}$ equal to the most expensive water source (assumed to be deionized water), $\$1.0$ $\$/\text{m}^3$.

$$C_{\text{water type}} = \frac{\sum_{i=1}^w (m_{\text{H}_2\text{O},i}^{\text{in}} \times C_{\text{H}_2\text{O},i})}{V_{\text{water, tot.}}} \quad (109)$$

12.28. Total solid waste cost, $C_{s \text{ tot.}}$. These are the costs related to the handling and disposal of solid waste produced during the day-to-day operation of a manufacturing plant: external waste removal fees, internal storage, personnel, waste treatment, and transportation costs. Equation (109) describes the calculation of this indicator. Where $C_{\text{solid treat.}}$ is the solid waste disposal cost, \$/kg. The best case scenario value is a zero $C_{s \text{ tot.}}$ moreover, a worst case scenario value is when all solid waste is categorized as hazardous with a $C_{s \text{ tot.}}$ unit cost of \$2/kg.

$$C_{s \text{ tot.}} = \sum_{j=1}^s (C_{\text{solid treat.},j} \times m_{\text{solid w.},j}^{\text{out}}) \quad (109)$$

12.29. Solid waste cost fraction, $C_{s \text{ spec.}}$. These are the costs related to the handling and disposal of solid waste produced during the day-to-day operation of a manufacturing plant normalized by the total production cost. Equation (109) describes the calculation of this indicator. The best case scenario value is zero and a worst case scenario value is when all solid waste is categorized as hazardous with a $C_{s \text{ tot.}}$ unit cost of \$2/kg divided by $\text{TPC}_{\text{worst-case}}$.

$$C_{s \text{ spec.}} = \frac{\sum_{j=1}^s (C_{\text{solid treat.},j} \times m_{\text{solid w.},j}^{\text{out}})}{\text{TPC}} \quad (109)$$

12.30. Total liquid waste cost, $C_{l \text{ tot.}}$. These are the costs related to the handling of liquid waste produced during the day-to-day operation of a manufacturing plant: external waste removal fees, internal storage, personnel, waste treatment, and transportation costs. Equation (109) describes the calculation of this indicator. Where $C_{\text{liquid treat.}}$ is the liquid waste disposal cost, \$/kg. The best case scenario value is a zero $C_{l \text{ tot.}}$ and a worst case scenario value is when all liquid waste is categorized as hazardous with a $C_{l \text{ tot.}}$ unit cost of \$2/kg.

$$C_{l \text{ tot.}} = \sum_{j=1}^l (C_{\text{liquid treat.},j} \times m_{\text{liquid w.},j}^{\text{out}}) \quad (109)$$

12.31. Liquid waste cost fraction, $C_{l \text{ spec.}}$. These are the costs related to the handling of liquid waste produced during the day-to-day operation of a manufacturing plant

normalized by the total production cost. Equation (109) describes the calculation of this indicator. The best case scenario value is zero and a worst case scenario value is when all liquid waste is categorized as hazardous with a $C_{l \text{ tot.}}$ unit cost of \$2/kg divided by $TPC_{\text{worst-case}}$.

$$C_{l \text{ spec.}} = \frac{\sum_{j=1}^l (C_{\text{liquid treat.},j} \times m_{\text{liquid w.},j}^{\text{out}})}{TPC} \quad (109)$$

12.32. Costs of purifying air, $C_{\text{pur. air}}$. These are the costs related to the handling of air releases produced during the operation of a manufacturing plant: external waste removal fees, internal storage, personnel, waste treatment, and transportation costs. Equation (109) describes the calculation of this indicator. Where $C_{\text{air pur.}}$ is the air purification cost, \$/kg. The best case scenario value is a zero $C_{\text{air pur.}}$ moreover, a worst case scenario value is when all air emissions are categorized as hazardous with a $C_{\text{air pur.}}$ unit cost of \$2/kg.

$$C_{\text{pur. air}} = \sum_{j=1}^a (C_{\text{air pur.},j} \times m_{\text{air w.},j}^{\text{out}}) \quad (109)$$

12.33. Fractional costs of purifying air, $C_{\text{pur. air fract.}}$. These are the costs related to the handle of air releases normalized by the total production cost. Equation (109) describes the calculation of this indicator. The best case scenario value is zero and a worst case scenario value is when all liquid waste is categorized as hazardous with a $C_{\text{air pur.}}$ unit cost of \$2/kg divided by $TPC_{\text{worst-case}}$.

$$C_{\text{pur. air fract.}} = \frac{\sum_{j=1}^a (C_{\text{air pur.},j} \times m_{\text{air w.},j}^{\text{out}})}{TPC} \quad (109)$$

VIII. Indicator Result Data and Plots

A biodiesel manufacturing process was selected as the case study for implementing the GREENSCOPE sustainability evaluation and design tool. An alkali-catalyzed transesterification reaction was considered for the manufacturing of biodiesel (FAME) and a complete steady state process simulation was performed. A complete and detailed description of this biodiesel process sustainability evaluation, its simulation, and characteristics are described in Ruiz-Mercado et al. (2013).¹ A core contribution of the GREENSCOPE process evaluation tool is the ability to define

and calculate the best case and worst case limits for each of the ~140 indicators. Calculation of all of the GREENSCOPE indicators was performed after completion of all data requirements. The results obtained for this simulated biodiesel manufacturing process were illustrated on radar diagrams for each of the sustainability bases. Figure 17 describes the environmental indicator results, and a full list of economic indicator results, worst and best case values, and dimensionless sustainability scores are collected in Table 1. The center of the radar graph represents a zero sustainability value (i.e., worst-case scenario) and the external boundary of the graph represents a 100% sustainability value (i.e., best-case scenario). The worst and best case scenario values were calculated as explained in section 10. The results for many of the environmental sustainability indicators, as described in Figure 17, represent a high level of sustainability and are indicative of good process performance for many environmental aspects. However, there are some critical aspects related to solid releases as reflected in some of the indicator scores (see Table 1 indicators no. 52–57, 59, 60).

On the other hand, the majority of the efficiency indicators employ input/output process material flows and their respective chemical reaction data. Figure 18 depicts on a radar diagram the individual scores of all efficiency based sustainability indicators. Table 2 shows all indicator results, reference values, and percentage scores. By setting these boundary limits for each indicator, the corresponding indicator value can be calculated as a percent sustainability value. This value now allows for a direct assessment of a chemical process for its own sustainability status and for assessing how far the process is from achieving a more desirable sustainable state.

The energy sustainability indicator results (see Figure 19) describe a thermodynamic process analysis that is primarily based on conventional energy balances and exergy analysis. For this case study, it was assumed any energy supplied to the process such as electricity, steam, and cooling water was generated from nonrenewable energy sources. Upon completing this sustainability evaluation, energy improvement opportunities have been identified in the energy indicator scores (see Table 3).

The economic results detail both profitability and costs (see Figure 20). In accordance with the procedure for computing these economic sustainability indicators, their results show a strong dependency on costs that are associated to the process inputs such as feedstocks and energy utilities. A full list of economic indicator results, worst and best-case values, and dimensionless sustainability scores are collected in Table 4.

Finally, this user's guide explains with details the procedure to implement a sustainability evaluation with the GREENSCOPE tool. The sustainability indicators, their data entries and their results are explained in this document. In addition, it is demonstrated the practicability and robustness of the GREENSCOPE tool for process sustainability evaluation during the manufacturing of biodiesel. This practical guide demonstrates the indicators and their realistic

measurement scales can quantitatively measure the sustainability level for any chemical process without falling into ambiguous definitions or qualitative aspects of sustainability. Therefore, GREENSCOPE is proposed and demonstrated as a reliable and powerful tool for sustainability evaluations and has the potential to aid in the development and optimization of chemical processes to increase their sustainability.

Disclaimer

The U.S. Environmental Protection Agency through its Office of Research and Development (ORD) conducted the in-house research described here. It has not been subject to Agency review and therefore does not necessarily reflect the views of the Agency. No official endorsement should be inferred.

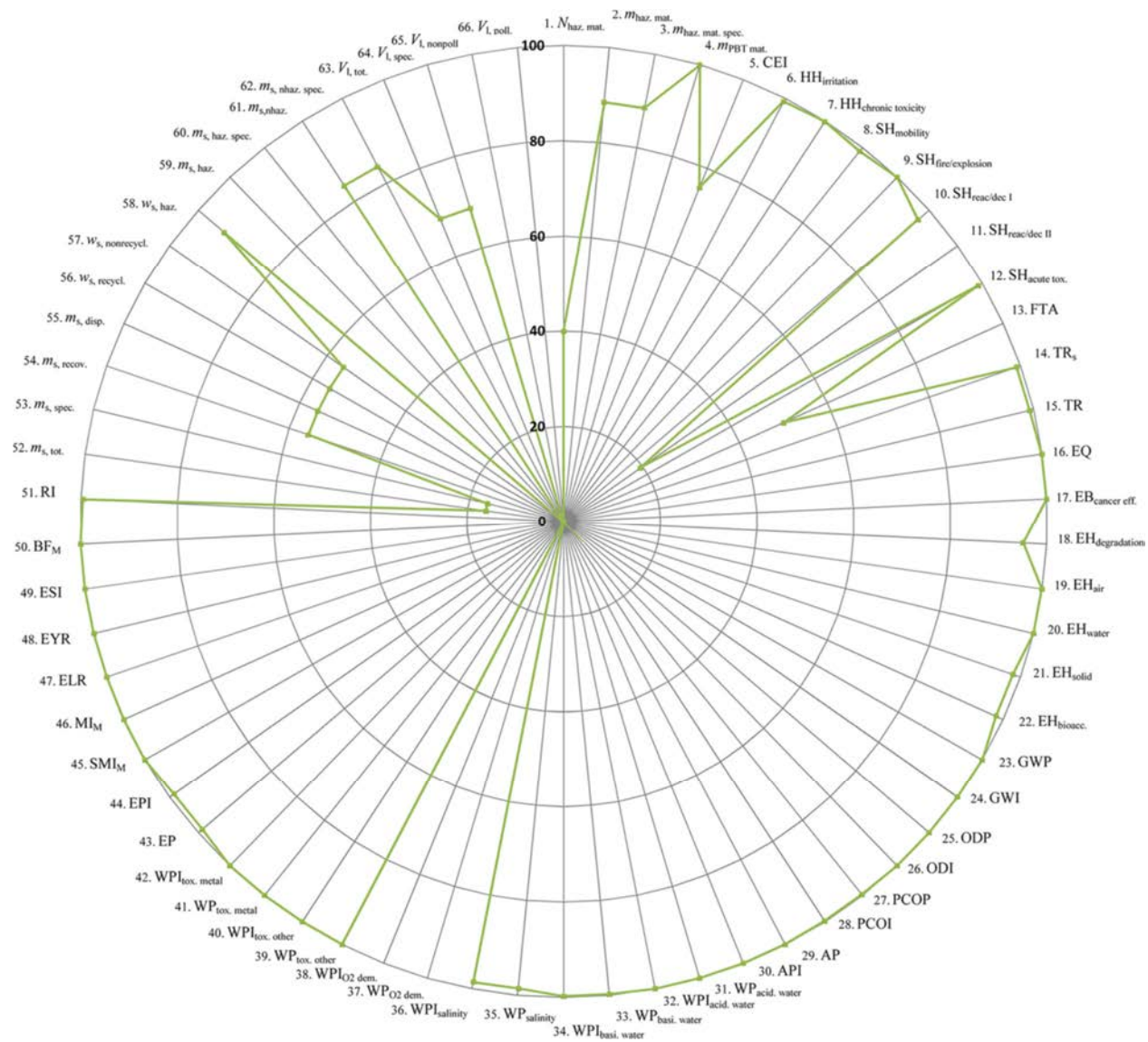


Figure 17. GREENSCOPE environmental indicator results for the simulated alkali-catalyzed manufacture of biodiesel.

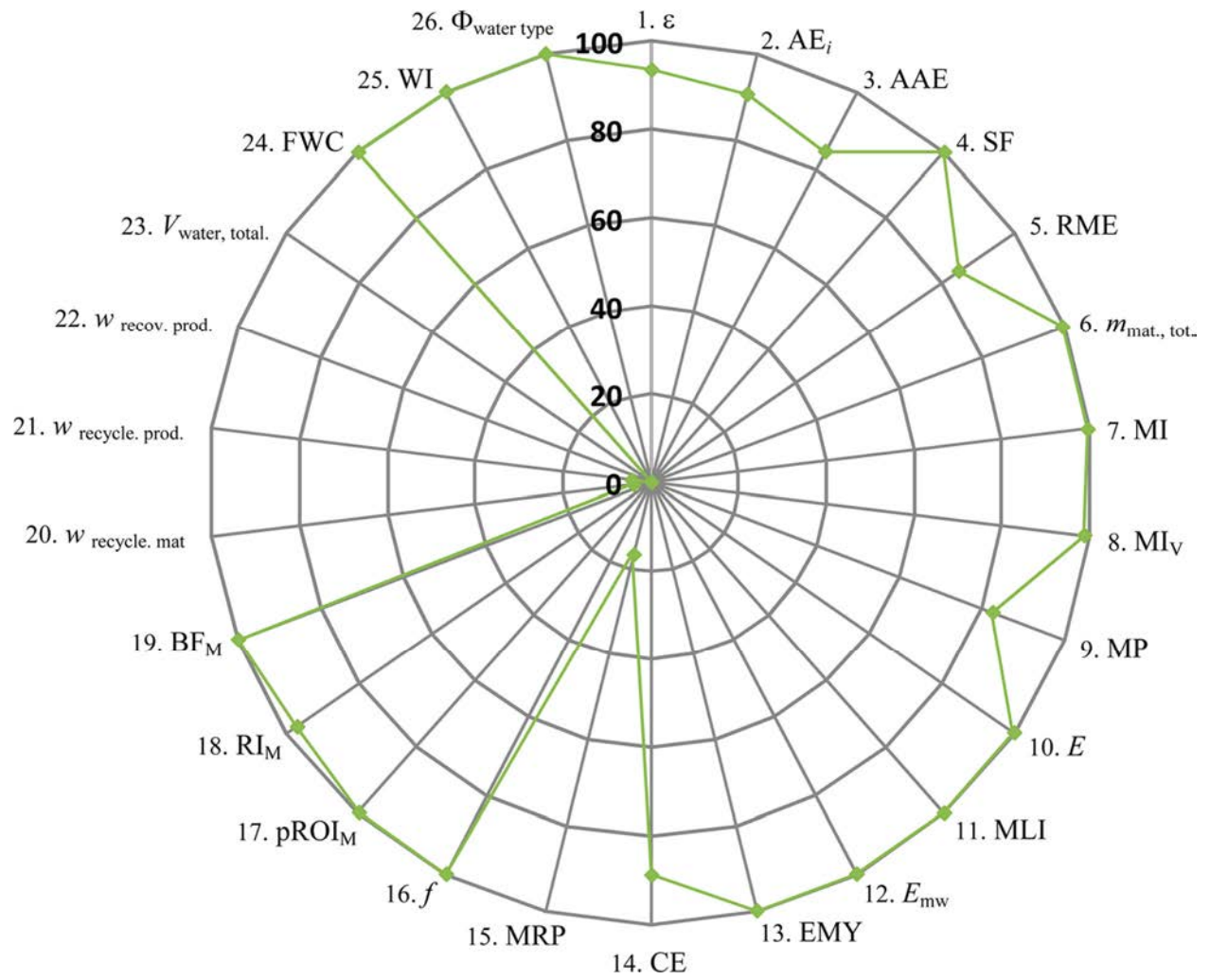


Figure 18. GREENSCOPE (material) efficiency indicator results for the simulated alkali-catalyzed manufacture of biodiesel.

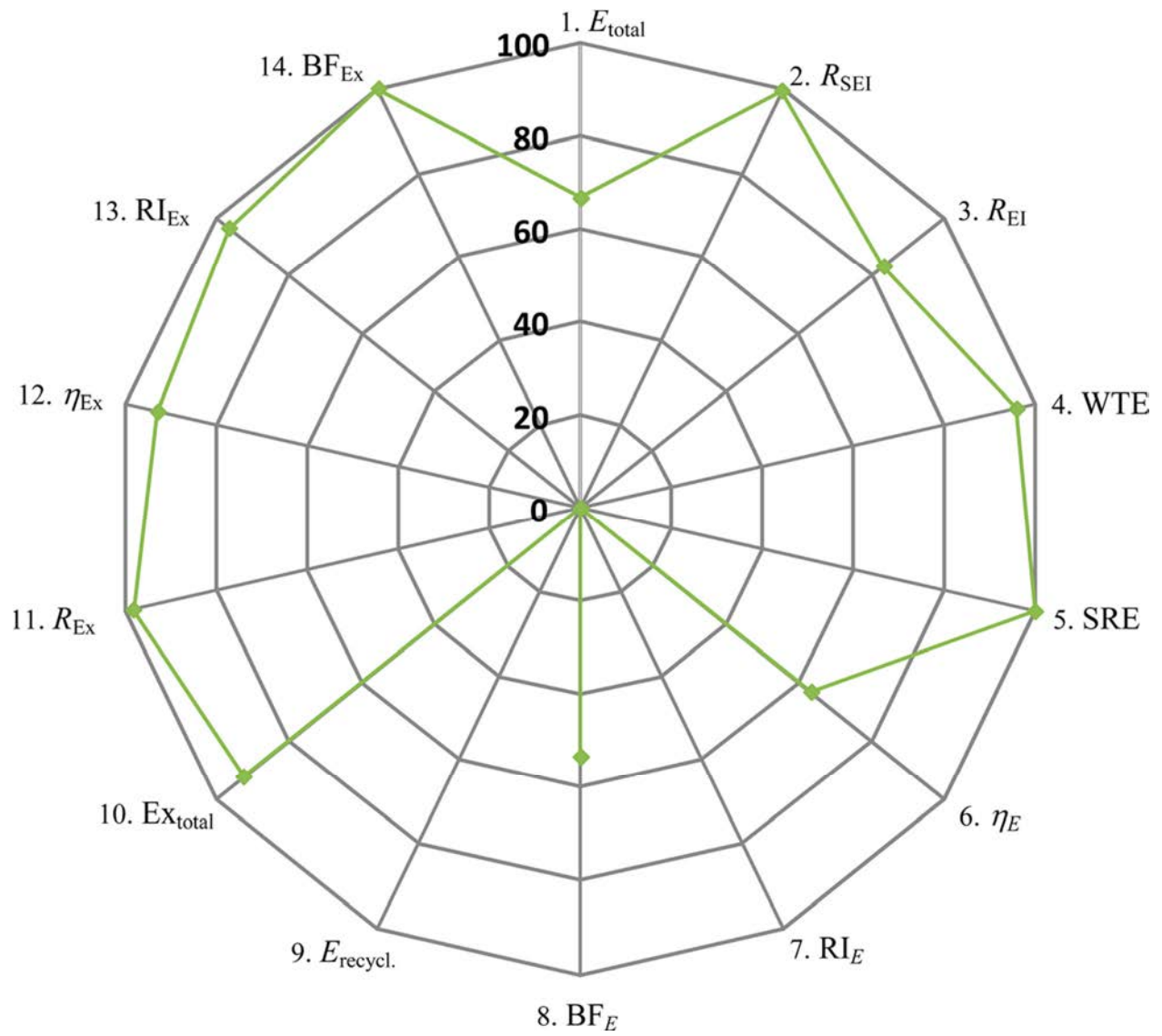


Figure 19. GREENSCOPE energy indicator results for the simulated alkali-catalyzed manufacture of biodiesel.

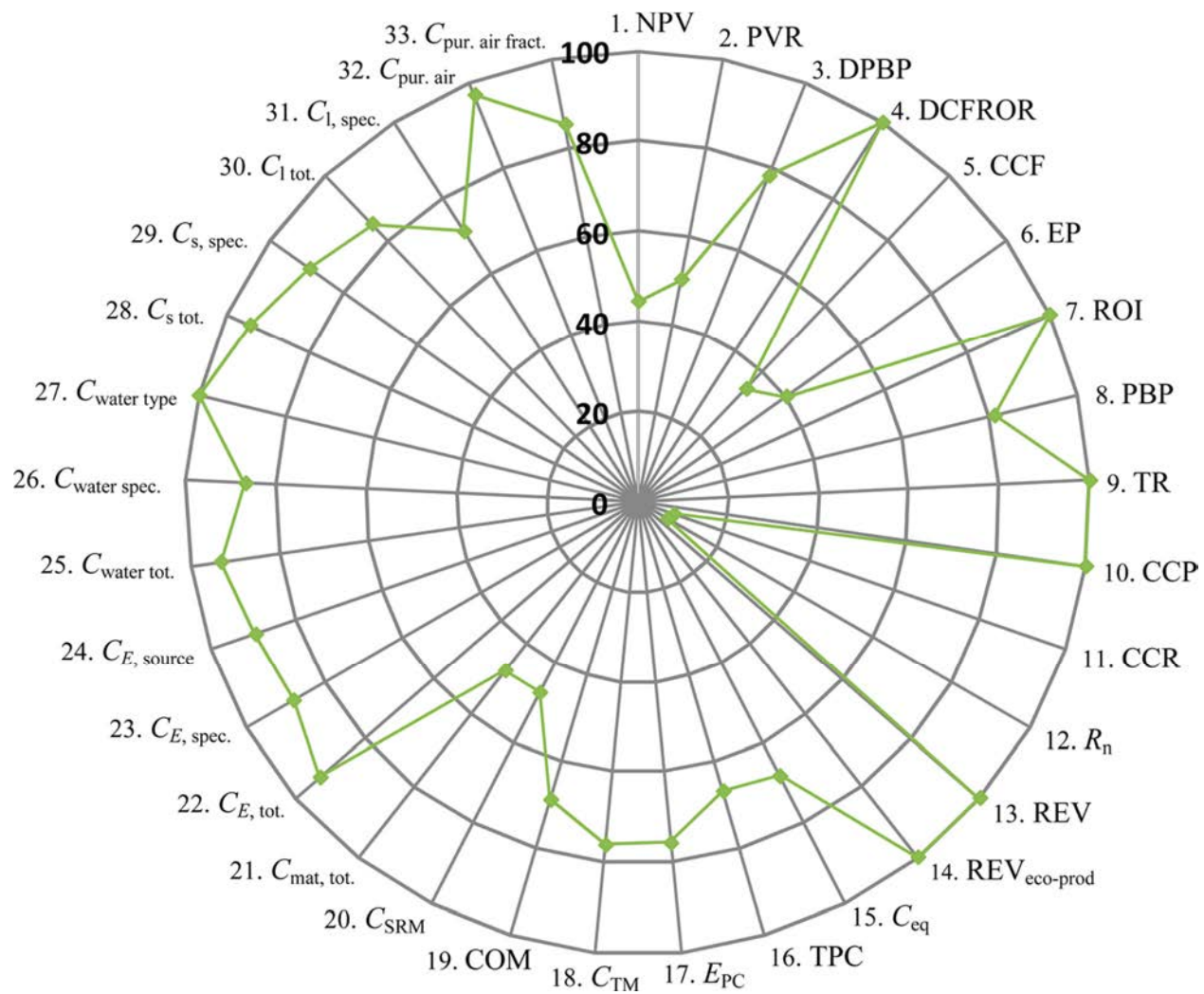


Figure 20. GREENSCOPE economic indicator results for the simulated alkali-catalyzed manufacturing of biodiesel.

Table 1. Environmental Indicators calculated for the simulated alkali-catalyzed manufacturing of biodiesel.

Indicator	Description	Unit	Worst-case	Best-Case	Calculated Value	Sust. (%)
1. $N_{\text{haz. mat.}}$	Number of hazardous materials input	dimensionless	5	0	3	40
2. $m_{\text{haz. mat.}}$	Mass of hazardous materials input	kg/h	1198.200	0	137.2000	88.55
3. $m_{\text{haz. mat. spec.}}$	Specific hazardous raw materials input	kg hazardous input/kg product	1.095	0	0.1254	88.55
4. $m_{\text{PBT mat.}}$	Total mass of persistent, bio-accumulative and toxic chemicals used	kg/h	1198.200	0	0	100
5. CEI	Chemical exposure index	dimensionless	1000	0	242.9911	75.70
6. $\text{HH}_{\text{irritation}}$	Health hazard, irritation factor	m^3/kg	1.000E+06	0	6893.3021	99.31
7. $\text{HH}_{\text{chronic toxicity}}$	Health hazard, chronic toxicity factor	m^3/kg	1.000E+07	0	9872.3701	99.90
8. $\text{SH}_{\text{mobility}}$	Safety hazard, mobility	kg/kg prod	10	0.0001	0.0934	99.07
9. $\text{SH}_{\text{fire/explosion}}$	Safety hazard, fire/explosion	kJ/kg prod	8.331E+07	0	3523.9177	100
10. $\text{SH}_{\text{reac/dec I}}$	Safety hazard, reaction / decomposition I	1	1	0	0.0300	97
11. $\text{SH}_{\text{reac/dec II}}$	Safety hazard, reaction / decomposition II	kJ/kg prod	3831.151	0	3084.9074	19.48
12. $\text{SH}_{\text{acute tox.}}$	Safety hazard, acute toxicity	m^3/kg	1.000E+05	0	953.2333	99.05
13. FTA	Fault tree assessment		0	1	0.5000	50
14. TR_s	Specific toxic release	kg/kg prod	0.982	0	0.0079	99.19
15. TR	Toxic release intensity	kg/US \$	0.614	0	0.0050	99.19
16. EQ	Environmental quotient	m^3/kg	19500	0	12.4258	99.94
17. $\text{EB}_{\text{cancer eff.}}$	Human health burden, cancer effects	kg/ US \$	0.614	0	0	100
18. $\text{EH}_{\text{degradation}}$	Environmental hazard, persistency of organic substances	kg/kg prod	1	0	0.0485	95.15
19. EH_{air}	Environmental hazard, air hazard	m^3/kg	1.000E+07	0	9872.3701	99.90
20. EH_{water}	Environmental hazard, water hazard	kg/kg prod	1.000E+05	0	31.0457	99.97

21. EH _{solid}	Environmental hazard, solid waste (inorganic pollutants)	kg/kg prod	1	0	0.0168	98.32
22. EH _{bioacc.}	Environmental hazard, bioaccumulation (the food chain or in soil)	kg/kg prod	100	0	1.6569	98.34
23. GWP	Global warming potential	kg CO ₂ equivalent/kg prod	0.9817	0	0	100
24. GWI	Global warming intensity	kg CO ₂ equivalent/US \$	0.6137	0	0	100
25. ODP	Stratospheric ozone-depletion potential	kg CFC-11 equivalent/kg prod	0.9817	0	0	100
26. ODI	Stratospheric ozone-depletion intensity	kg CFC-11 equivalent/ US \$	0.6137	0	0	100
27. PCOP	Photochemical oxidation (smog) potential	kg Ethylene equivalent/kg prod	0.9754	0	0.0016	99.83
28. PCOI	Photochemical oxidation (smog) intensity	kg Ethylene equivalent/ US \$	0.6098	0	0.001	99.84
29. AP	Atmospheric acidification potential	kg SO ₂ equivalent/time	0.9817	0	0	100
30. API	Atmospheric acidification intensity	kg SO ₂ equivalent/US \$	0.6137	0	0	100
31. WP _{acid. water}	Aquatic acidification potential	kg H ⁺ equivalent/time	0.9641	0	0.0002	99.98
32. WPI _{acid. water}	Aquatic acidification intensity	kg H ⁺ equivalent/US\$	0.6028	0	0.0001	99.98
33. WP _{basi. water}	Aquatic basification potential	kg OH ⁻ released/time	0.9670	0	0.0025	99.74
34. WPI _{basi. water}	Aquatic basification intensity	kg OH ⁻ released/US \$	0.6046	0	0.0016	99.74
35. WP _{salinity}	Aquatic salinization potential	kg Salt-forming ion equivalent/time	0.9677	0	0.0141	98.54
36. WPI _{salinity}	Aquatic salinization intensity	kg Salt-forming ion equivalent/US \$	0.6050	0	0.0088	98.55
37. WP _{O₂ dem.}	Aquatic oxygen demand potential	kg O ₂ equivalent/time	2.7796	0	2.7628	0.60
38. WPI _{O₂ dem.}	Aquatic oxygen demand intensity	kg O ₂ equivalent/US \$	1.7378	0	1.7273	0.60
39. WP _{tox. other}	Ecotoxicity to aquatic life potential	kg formaldehyde equivalent/time	0.9704	0	0	100
40. WPI _{tox. other}	Ecotoxicity to aquatic life intensity	kg formaldehyde equivalent/US \$	0.6067	0	0	100
41. WP _{tox. metal}	Ecotoxicity to aquatic life potential by metals	kg Cu equivalent/time	0.9704	0	0	100
42. WPI _{tox. metal}	Ecotoxicity to aquatic life intensity by metals	kg Cu equivalent/time	0.6067	0	0	100
43. EP	Eutrophication potential	kg PO ₄ ³⁺ equivalent/time	0.9702	0	0.0108	98.89

Table 2. Efficiency indicators calculated for the simulated alkali-catalyzed manufacturing of biodiesel.

44. EPI	Eutrophication potential intensity	kg PO ₄ ³⁺ equivalent/US \$	0.6065	0	0.0067	98.90
45. SMI _M	Specific emery intensity	MseJ/kg of prod	5.393E+08	5.3932E+07	5.2604E+07	100
46. MI _M	Emery intensity	MseJ/ US \$	6.115E+08	3.3718E+07	3.2888E+07	100
47. ELR	Environmental loading ratio	MseJ/MseJ	10	2	0.0046	100
48. EYR	Emery yield ratio	scalar, 0 to ∞+	0	1	1.0773	100
49. ESI	Emery sustainability Index	scalar	1	5	233.8457	100
50. BF _M	Breeding factor	fraction	0	10	234.9230	100
51. RI	Renewability index	fraction	0	1	0.9954	99.54
52. <i>m_{s, tot.}</i>	Total solid waste mass	kg	83.011	0	69.5645	16.20
53. <i>m_{s, spec.}</i>	Specific solid waste mass	kg/kg prod	0.076	0	0.0636	16.20
54. <i>m_{s, recov.}</i>	Solid waste mass for recovery	kg	0	69.5645	38.8839	55.90
55. <i>m_{s, disp.}</i>	Solid waste mass for disposal	kg	69.565	0	30.6806	55.90
56. <i>w_{s, recycl.}</i>	Recycling mass fraction	kg/kg solid releases	0	1	0.5590	55.90
57. <i>w_{s, non-recycl.}</i>	Disposal mass fraction	kg/kg solid releases	1	0	0.4410	55.90
58. <i>w_{s, haz.}</i>	Hazardous solid waste mass fraction	kg hazard solid/kg solid releases	1	0	0.0709	92.91
59. <i>m_{s, haz.}</i>	Total hazardous solid waste disposal	kg hazardous solid releases	4.929	0	4.9288	0
60. <i>m_{s, haz. spec.}</i>	Specific hazardous solid waste	kg non-hazard solid/kg prod	4.505E-03	0	0.0045	0
61. <i>m_{s, n-haz.}</i>	Total non-hazardous solid waste disposal	kg non-hazardous solid	0	30.6806	25.7518	83.94
62. <i>m_{s, n-haz. spec.}</i>	Non-hazardous solid waste intensity	kg non-hazardous solid/US \$	0	0.0175	0.0147	83.94
63. <i>V_{l, tot.}</i>	Total volume of liquid waste	m ³ /h	0.079	0	0.0247	68.64
64. <i>V_{l, spec.}</i>	Specific liquid waste volume	m ³ /kg prod	7.197E-05	0	2.2570E-05	68.64
65. <i>V_{l, non-poll.}</i>	Non-polluted liquid waste volume	m ³	0	0.0247	0	0
66. <i>V_{l, poll.}</i>	Polluted liquid waste volume	m ³	0.025	0	0.0247	0

Indicator	Description	Unit	Worst-case	Best-case	Calculated Value	Sust. (%)
1. ϵ	Reaction yield	kg/kg	0	1	0.935	93.50
2. AE _i	Atom economy	kg/kmol / kg/kmol	0	1	0.906	90.60
3. AAE	Actual atom economy	kg/kmol / kg/kmol	0	1	0.847	84.70
4. SF	Stoichiometric factor	kg/kg	41	1	1.003	99.99
5. RME	Reaction mass efficiency	kg/kg	0	1	0.845	84.50
6. <i>m_{mat., tot.}</i>	Total material consumption	kg/h	39600	990	1198.200	99.46

7. MI_v	Value mass intensity	kg/kg	40	1	1.210	99.46
8. MI	Mass intensity	kg/\$	52	0	0.685	98.68
9. MP	Mass productivity	kg/kg	0	1	0.826	82.60
10. E	Environmental factor	kg/kg	39	0	0.084	99.78
11. MLI	Mass loss index	kg/kg	100	0	0.095	99.91
12. E_{mw}	Environmental factor based on molecular weight	kg/kmol / kg/kmol	100	0	0.104	99.90
13. EMY	Effective mass yield	kg/kg	40	0	7.216	99.65
14. CE	Carbon efficiency	kmol/kmol	0	1	0.887	88.70
15. MRP	Material recovery parameter	kg/kg	0	1	0.167	16.70
16. f	Solvent and catalyst environmental impact parameter	kg/kg	62	0	0.031	99.95
17. $pROI_M$	Physical return on investment	kg/kg	40	0	10.526	99.76
18. RI_M	Renewability-material index	kg/kg	0	1	0.974	97.40
19. BF_M	Breeding-material factor	kg/kg	0	10	38.652	100
20. $w_{recycl. mat.}$	Recycled material fraction	kg/kg	0	1	0.041	4.10
21. $w_{recycl. prod.}$	Mass fraction of product from recyclable materials	kg/kg	0	1	0.045	4.50
22. $w_{recov. prod.}$	Mass fraction of product designed for disassembly, reuse or recycling	kg/kg	0	1	7.531E-06	0
23. $V_{water, tot.}$	Total water consumption	m ³ /h	0.01	0	0.011	0
24. FWC	Fractional water consumption	m ³ /kg	2.95	0	1.005E-05	100
25. WI	Water intensity	m ³ /US \$	1.55	0	6.285E-06	100
26. $\Phi_{water type}$	Volume fraction of water type	m ³ /m ³	1	0	0	100

Table 3. Energy indicators calculated for the simulated alkali-catalyzed manufacturing of biodiesel.

Indicator	Description	Unit	Worst-case	Best-case	Calculated Value	Sust. (%)
1. E_{total}	Total energy consumption	MJ/h	27401.00	2740.10	10964.7269	66.65
2. R_{SEI}	Specific energy intensity	MJ/kg	1949.00	0.00	10.0213	99.49
3. R_{EI}	Energy intensity	MJ/US \$	37.30	0.00	6.2652	83.20
4. WTE	Waste treatment energy	MJ/kg	1	0.00	0.0407	95.94
5. SRE	Solvent recovery energy	MJ/kg	1	0.00	0.0000	100
6. η_E	Resource-energy efficiency	fraction	0	1.00	0.6316	63.26
7. RI_E	Renewability-energy index	fraction	0	1.00	0.0000	0
8. BF_E	Breeding-energy factor	scalar	0	10.00	5.3382	53.38
9. $E_{recycl.}$	Energy for recycling	MJ/kg	1.00	0.00	3.0661	0
10. Ex_{total}	Exergy consumption	MJ/h	42962.62	0.00	3178.2118	92.59
11. R_{Ex}	Exergy intensity	MJ/kg	196.33	39.27	41.6397	98.48
12. η_{Ex}	Resource-exergy efficiency	fraction	0	1.00	0.9311	93.10
13. RI_{Ex}	Renewability-exergy index	scalar	0	1.00	0.9654	96.54
14. BF_{Ex}	Breeding-exergy factor	fraction	0	10.00	26.9335	100

Table 4. Economic indicators calculated for the simulated alkali-catalyzed manufacturing of biodiesel.

Indicator	Description	Unit	Worst-case	Best-case	Calculated Value	Sust. (%)
1. NPV	Net present value	1×10 ⁶ US \$	0.16632	7.58479	3.46880	44.52
2. PVR	Present value ratio	\$/ \$	1	4.72935	2.87613	50.31
3. DPBP	Discounted payback period	Yr	11	1	3.21000	77.90
4. DCFROR	Discounted cash flow rate of return	%	0	40	41.60000	100
5. CCF	Capital charge factors	1/yr	0	1	0.34617	34.62
6. EP	(Specific) Economic potential	US \$/kg product	0	1	0.40244	40.24
7. ROI	Rate of return on investment	fraction or %	0	0.4	0.52888	100
8. PBP	Payback Period	Yr	11	1	2.89000	81.10
9. TR	Turnover ratio	\$/ \$	0.2	4	8.67463	100
10. CCP	Cumulative cash position	1×10 ⁶ US \$	0	1.76853	7.58479	100
11. CCR	Cumulative cash ratio	\$/ \$	0	56.61523	4.72935	8.35
12. R _n	Net return	1×10 ⁶ US \$/yr	0	58.08070	4.33070	7.46
13. REV	Revenues from eco-products	1×10 ⁶ US \$/yr	0	15.34133	15.34133	100
14. REV _{eco-prod.}	Revenue fraction of eco-products	\$/ \$	0	1	1.00000	100
15. C _{eq}	Equivalent annual cost	1×10 ⁶ US \$	30.61448	6.88542	14.41193	68.28
16. TPC	Total product cost	1×10 ⁶ US \$/yr	34.14628	9.35060	17.60118	66.73
17. E _{PC}	Production cost	1×10 ⁶ US \$/yr	27.73945	3.63024	9.45992	75.82
18. C _{TM}	Capital cost	1×10 ⁶ US \$/yr	4.62470	0.87896	1.76853	76.25
19. COM	Manufacturing cost	1×10 ⁶ US \$/yr	30.25470	6.71042	14.08094	68.70
20. C _{SRM}	Specific raw material cost	US \$/ mass of product	1.46810	0.18351	0.85644	47.62
21. C _{mat, tot.}	Total material cost	1×10 ⁶ US \$/yr	14.08094	1.76012	8.21437	47.62
22. C _{E, tot.}	Total energy cost	1×10 ⁶ US \$/yr	4.03531	0.04131	0.31655	93.11
23. C _{E, spec.}	Specific energy costs	\$/ \$	0.11818	0.00442	0.01798	88.07
24. C _{E, source}	Average cost of energy source	US \$/MJ	0.01680	0.00172	0.00329	89.57
25. C _{water tot.}	Total water cost	US \$/yr	96.42600	0	6.46054	93.30
26. C _{water spec.}	Water cost fraction	\$/ \$	2.8239E-06	0	0.00000	87
27. C _{water type}	Average volume water type cost	US \$/m ³ water	1	0.06700	0.06700	100
28. C _{s tot.}	Total solid waste cost	1×10 ⁶ US \$/yr	1.21960	0	0.06792	94.43
29. C _{s spec.}	Solid waste cost fraction	\$/ \$	0.03572	0	0.00386	89.20
30. C _{l tot.}	Total liquid waste cost	1×10 ⁶ US \$/yr	0.50692	0	0.07492	85.22
31. C _{l spec.}	Liquid waste cost fraction	\$/ \$	0.01485	0	0.00426	71.33
32. C _{pur. air}	Costs of purifying air	1×10 ⁶ US \$/yr	2.22329	0	0.06225	97.20
33. C _{pur. air fract.}	Fractional costs of purifying air	\$/ \$	0.02400	0	0.00354	85.26

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