ESTIMATe – Early STage IMpact Assessment Tool

User Manual

Intended Use of ESTIMATe

ESTIMATe facilitates early-stage Life-Cycle Assessment (LCA) of CO_2-based chemicals for non-LCA experts. For this purpose, LCA methodology and data generation are automated where possible. ESTIMATe is not intended to replace conventional LCA studies, but rather to allow considering an environmental perspective earlier in process development before LCA specialists are usually consulted.

ESTIMATe was developed for Excel for Microsoft 365. Compatibility issues might arise with earlier Excel versions.

Copyright

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Table of Contents

Part 1: Practical Manual

1. Structure of the ESTIMATe tool

The following Worksheets exist in the ESTIMATe Excel Workbook:

Overview

- The overview sheet contains information on authors, licensing terms, and references.

New Assessment

- New assessments are created here.

Assessment Sheets

- Each assessment in ESTIMATe "lives" on its own sheet. This assessment sheet comprises the study setup, data generation, calculation, and result visualization.
- As the basis for new assessments, ESTIMATe includes three assessment sheet templates: *Best_Case_Assessment_template, Hotspot_Assessment_template,* and *MPA_template*. These template sheets are hidden by default.

Background Data Sheets

- Estimate uses chemical property data and life-cycle impact data for calculations. Four background data sheets are used:
  1. chemicals
     - Contains substance and property data on chemical intermediates.
     - Also contains information required for LCA calculations where such information is available, such as
       - Impact factors upon emission of the substance to the environment
       - Connected background process from *data_ei* or scenarios to characterize the environmental impacts of chemical production.
  2. data_ei
     - Contains an abbreviated ecoinvent database with life-cycle impact data.
  3. scenarios
     - Contains life-cycle impact data on intermediates for which decarbonization scenarios are applied in ESTIMATe.
     - Specifically, ESTIMATe applies decarbonization scenarios for feedstock carbon dioxide, hydrogen, electricity, heat, steam, and methane/natural gas.
  4. data_own
     - Contains life-cycle impacts and assumptions for user-created process.
     - The user may save all assumptions and results of assessments to data_own. This allows the use of the process as a background process in future assessments.
  5. impact categories
     - Contains metadata on impact assessment categories, including name, unit, and overarching method.

New mixture

- In the new mixture sheet, the user may define a mixture as a weighted average of individual substance properties. The mixture is added to the *chemicals* sheet. The new mixture feature is mainly intended to allow assessing fuels. The sheet is hidden by default and can be accessed through the *New Mixture* sheet.

Estimation methods

- Estimation methods may be used to close data gaps in early-stage assessments.
- The estimation method allows application of estimation methods and offers an explanation with each method.

Processes, DropDown, and Figures

- These auxiliary Worksheets are used for dropdown menu and figure creation. These three sheets are hidden by default.

Most of the calculations in ESTIMATe run in Excel VBA. Users generally do not need to directly interact with the code. However, you may refer to the Technical Manual section of this manual for the documentation of the individual functions and info on how to access them.

2. Setting up the ESTIMATe tool

The following set up needs to be performed only once after download of the ESTIMATe tool. ESTIMATe relies on the ecoinvent database[1] for life-cycle impact data, which are commercially available and thus cannot be included in ESTIMATe.

An ecoinvent license is required for the full functionality of ESTIMATe.

To import the ecoinvent database into the ESTIMATe tool, perform the following steps:

1. Download the database in .xlsx Format from the ecoinvent website.

   Ecoinvent is offered in multiple versions ("system models") differing slightly in background modeling assumptions. ESTIMATe was designed using ecoinvent 3.8 cut-off. Adaptations might be necessary to import other versions of ecoinvent (cf. Section 10.1).

   1. Log in to the ecoinvent website using your credentials.
   2. Navigate to the "Files" tab.
   3. Under "Allocation cut-off by classification" click on the file with the ending "cumulative_**lcia_xlsx**.7z" to start the download.
   4. Unpack the xlsx file from the zip folder.

2. Bring data into the correct format for ESTIMATe.
   1. Place the unpacked .xlsx ecoinvent file into the same folder in which "import_ecoinvent.xlsx" is located.
   2. Open the "import_ecoinvent.xlsx" Excel file that is provided with the ESTIMATe tool (cf. Figure 1).
   3. In "import_ecoinvent.xlsx", specify the name of the ecoinvent database file you want to import.
   4. Check the box "Calculate scenario tables".
   5. Click "Start Import". The "import_ecoinvent.xlsx" will now shorten the ecoinvent database to products required for ESTIMATe. Then, a filtered ecoinvent sheet is created in the format that ESTIMATe expects. Furthermore, a "scenarios" sheet is created.

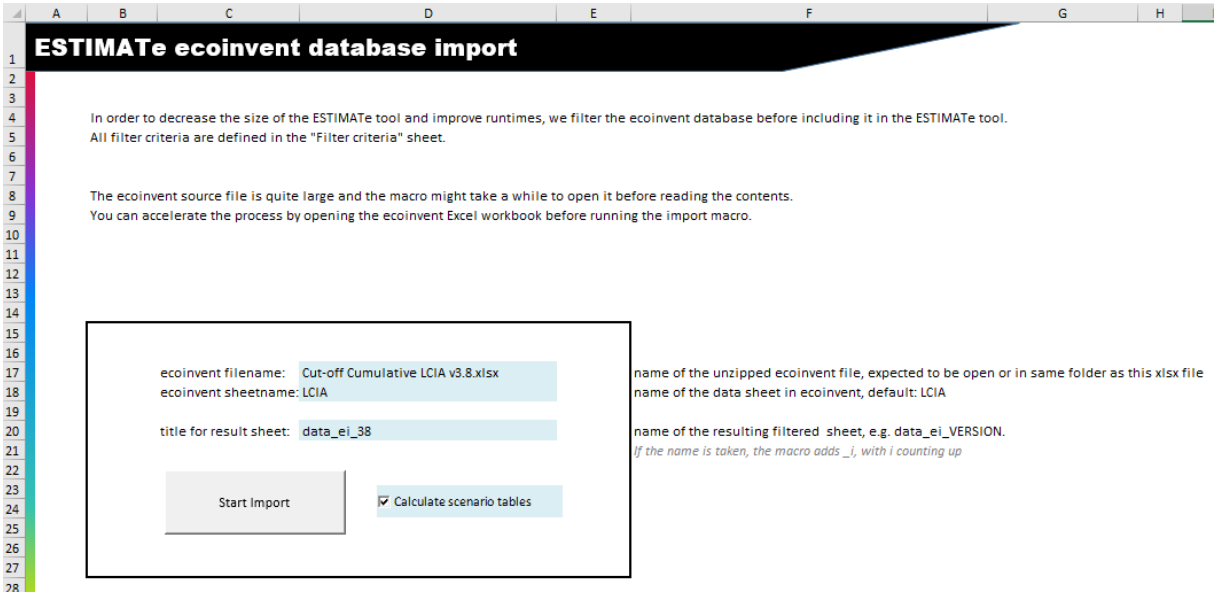


Figure 1: Exemplary input into the import_ecoinvent.xlsx file for ecoinvent import to ESTIMATe

3. Copy filtered ecoinvent data into ESTIMATe

Once the "import_ecoinvent.xlsx" has created the filtered ecoinvent datasheet, copy and paste all contents of the filtered sheet into the ESTIMATe tool "data_ei" sheet, replacing any data that might have existed there previously. To ensure the correct functioning of ESTIMATe, please double-check the following points:

- There is only one sheet called "data_ei" in ESTIMATe.xlsx.
- The "data_ei" sheet contains your imported data.
- The table on the "data_ei" sheet is called "table_data_ei" (check by selecting any cell within the table and then navigating to the "table" context menu at the top of the page)

4. Enter data on the "scenarios" sheet.

The "scenarios" sheet in ESTIMATe contains life-cycle impact data for key inputs of CCU chemical processes. For more information on scenarios, refer to the "scenarios" sheet or the ESTIMATe paper.

Copy the impact data from the *scenarios* sheet in the "import_ecoinvent.xlsx" file and paste into the *scenarios* sheet in ESTIMATe. Please copy and paste only the table contents, and mind that the tables in ESTIMATe have an extra column that is used for creating the figures to the left each tables. Do not overwrite this last column. To ensure the correct functioning of ESTIMATe, please double-check the following points:

- There is only one sheet called "scenarios" in ESTIMATe.xlsx.
- The "scenarios" sheet contains your imported data.
- The tables on the "scenarios" sheet are called (check by selecting any cell within the table and then navigating to the "table" context menu at the top of the page):
    - table_scen_co2
    - table_scen_hydrogen
    - table_scen_ng
    - table_scen_elec
    - table_scen_heat
    - table_scen_steam

You are all set to use ESTIMATe!

3. Starting a new assessment

Refer to Figure 2 for number references.

Choose a Study Goal [1].
There are three available goals explained on the right side [1a]. In the dropdown menu you can choose between Best-Case Assessment, Hotspot Assessment and Mitigation Potential Assessment.

Enter the name and short name of studied process [2].
The “name of the studied process” will be the title of your assessment and can be changed later.

The “short name”is the name of your assessment Excel sheet. The short name must be unique since it is used throughout the tool to identify the sheet and objects on it. You may not change the short name after creating the assessment since doing so will break the sheet. If an assessment with the same short name already exists, the new assessment cannot be created and you will be prompted to enter a different short name.

Choose the main product [3].
For Best-Case and Hotspot Assessments, you need to select the main product. All products that are listed in the *chemicals* sheet can be chosen in the dropdown menu. If you aim to assess a mixture, you may introduce a new mixture using the *New mixture* sheet before selecting a main product. A link to the *New mixture* sheet is located just next to the main product selection.

If the study goal “Mitigation Potential Assessment” is chosen, no main product must be selected since to existing assessments are compared.

Create a new assessment [4].
Click on the button “Create New Assessment” so that your new assessment sheet is created. If the button “Create New Assessment” is disabled, check whether the aforementioned steps were executed, macros are enabled, and all blue fields have a valid input.

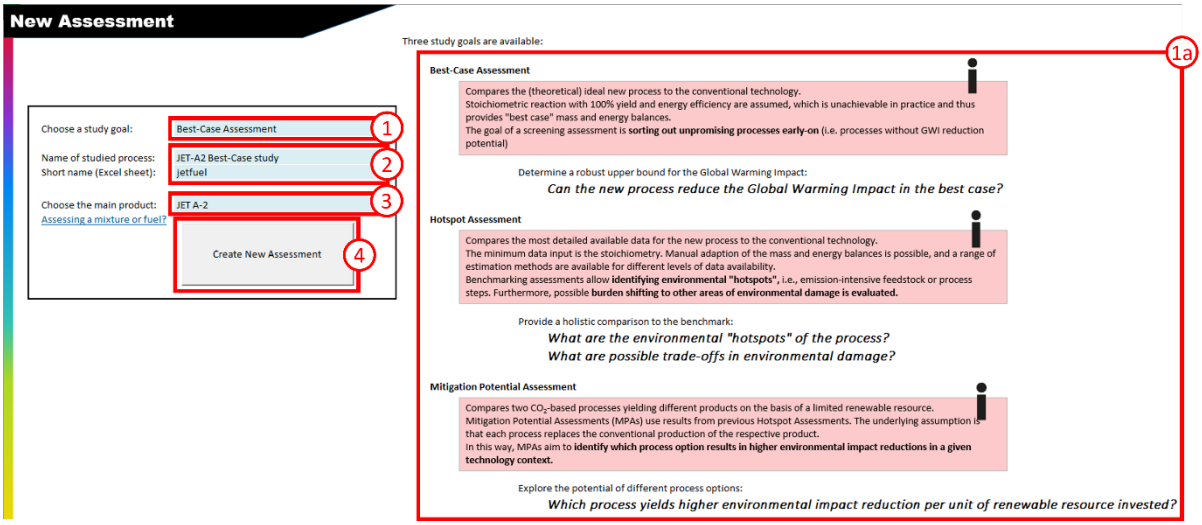


Figure 2: New Assessment sheet in the ESTIMATe tool, numbered for Click instructions

4. Conducting a Best-Case Assessment

4.1. Introduction: What is a Best-Case assessment?

Best-Case Assessments examine a theoretical ideal case of a CCU technology. By utilizing only theoretical best-case assumptions, the assessment establishes a robust lower boundary for the Global Warming Impact. Potential burden-shifting to other environmental impacts may also be investigated. The best-case environmental impacts are compared to those of a fossil-based benchmark process to answer the question “Can environmental impacts be mitigated in the best case?”. Essentially, Best-Case Assessments function as a sanity check, aiding in go/no-go decisions by offering a preliminary evaluation before embarking on process development.

4.2. Click instructions

For performing the Best-Case Assessment, you move through the sheet from top to bottom. The following Click Instructions are broken down into four sections: study setup, data generation, data check, and calculation with result presentation.

4.2.1. Study setup: Header of Best-Case Assessment

For this study setup section of instructions, the numbers in the text refer to Figure 3.

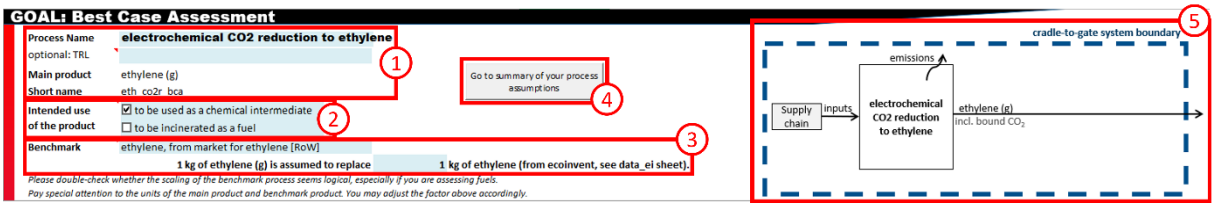


Figure 3: Header of an exemplary Best-Case Assessment in ESTIMATe

Review Assumptions and optionally specify a Technology Readiness Level (TRL) [1]
When creating a new Best-Case Assessment, process name, main product, and short name are directly filled in by the tool. [1] Please do not change the short name or sheet name since otherwise the code will not work anymore. You may, however, change the process name (blue cell). Optionally, you may enter a Technology Readiness Level (TRL). The TRL will be inserted into process assumptions and can help, e.g., in Mitigation Potential Assessments to evaluate technology comparability.

Review the intended use of the product and adapt if necessary [2]
Check the option which applies to your assessment: “to be used as a chemical intermediate” or “to be used as a fuel”. The intended use of the product serves to define the function of a product or process, which is an essential step in LCA. In ESTIMATe, it also determines the unit of the main product: the LCA study is scaled to 1 kg for intermediates, and to 1 MJ energy content for fuels. “To be used as a chemical intermediate” is the default selection when creating an assessment and user may select “to be incinerated as a fuel”

Review the benchmark process and scaling factor, especially when assessing fuels [3]

- Check whether the selected benchmark product makes sense in your assessment.
- Check whether the scaling factor is sensible, considering the unit of main product and benchmark.
- Repeat these checks whenever you change the intended use of your product!

Background information for step [3]:

The benchmark process impacts will be shown in the result figures to provide context for the CCU assessment results. If available, a default benchmark process is selected from the background database upon sheet creation. Default benchmarks are specified on the *chemicals* sheet. However, you may select any process from *data_ei*, *data_own*, or *scenarios* if it is more applicable to your case.

The scaling factor determines how much of the benchmark product is replaced by the product under study. The scaling factor is set to 1 when a benchmark is automatically set and "to be used as a chemical intermediate" is selected. For fuels, the scaling factor is set using the lower heating value of the assessed main product. Reasoning: most ecoinvent processes have a mass-based unit, e.g., 1 kg of kerosene. The scaling factor thus serves as a conversion factor between the energy content of a fuel product to the mass unit usually used in benchmark processes (using the lower heating value and molar mass of the main product).

Further elements of the header:

Go to summary of process assumptions [4]. At any point in your assessment, you may click the button to get to a summary of your process assumptions located right before the result figures of the assessment (cf. Section 4.2.4)

Overview of assessment system boundaries [5] updates as you make assumptions in ESTIMATe.

4.2.2. Data generation

For this data generation section of instructions, the numbers in the text refer to Figure 4.

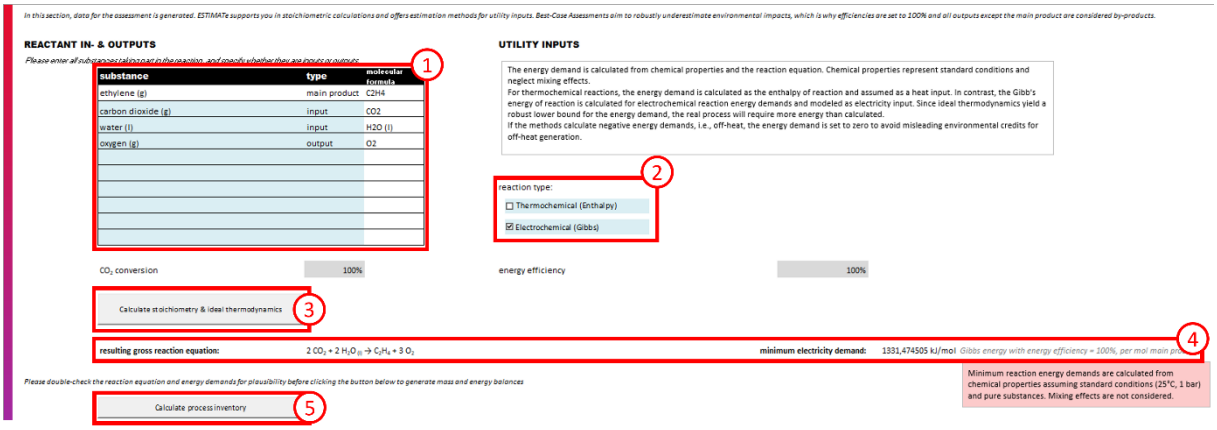


Figure 4: Exemplary data generation section in a Best-Case Assessment in ESTIMATe

Enter reactants to prepare the gross reaction equation [1]

Select all reactants in the substance column using dropdown menus and define them as inputs or outputs in the type column. Perfect CO_2 conversion (100%) is assumed for Best-Case Assessments and substance properties for calculations will be taken from the *chemicals* sheet.

Select a reactor type for energy demand calculations [2]

Check either the checkbox *thermochemical* or *electrochemical.* The energy demand will be calculated according to ideal thermodynamics:

- *thermochemical*: reaction enthalpy calculated & assumed as heat input.
- *electrochemical*: Gibb's energy calculated & assumed as electricity input.

In Best-Case Assessments, an ideal energy efficiency of 100% is assumed. If the energy demand is negative, it will be set to zero in the calculate process inventory step to avoid misleading environmental credits for, e.g., off-heat (see step [5]).

Click button to calculate brute reaction equation (stoichiometric) and minimum energy demand [3]

Check whether the resulting reaction equation and energy demand look sensible to you [4]
If the results look sensible, proceed. Otherwise, adapt your entries and recalculate ([1] to [3]).

Click button to calculate process inventory, i.e., mass and energy balances [5]
Upon the click, ESTIMATe calculates the "process inventory", i.e., a list of process mass and energy in- and outputs, and scales it to the main product unit as specified in the header (cf. "Intended use" in Section 4.2.1). The process inventory is entered into the table below the button.

4.2.3. Data check

For this data check section of instructions, the numbers in the text refer to Figure 5.

reference product	amount	unit	type (1)	linked process (2)
ethylene (g)	1	kg	main product	ethylene, from market for ethylene [RoW]
carbon dioxide (g)	3,1376	kg	input	ESTIMATe feedstock carbon dioxide
water (l)	1,2844	kg	input	water, deionised, from market for water, deionised [RoW]
oxygen (g)	3,4219	kg	emission	oxygen (g)
electricity	13,1840	kWh	input	ESTIMATe electricity

Figure 5: Exemplary process inventory of a Best-Case Assessment in ESTIMATe

Review the type [1] and connected background process [2] for each entry

- Check whether the linked process looks sensible.
- Check the type of your process outputs.

Background information on this step:

The process inventory table will already be filled with all relevant reference products and their corresponding amount, unit, type and, where available, linked process.

The following types are available: main product (filled in per default), input, by-product, and emission. Per default, all mass outputs assumed as emissions. If a substance would be considered a valuable by-product in a large-scale process, select "by-product" as type instead, and the environmental impact of the conventional production of the by-product is assumed avoided. This means your process will receive an environmental credit for avoiding conventional production.

The linked process provides a link to information on environmental impacts of the entry, either in the *chemicals* sheet (for emissions) or the *data_ei, data_own,* or *scenarios* sheets (for inputs, by-products, and wastes). For inputs where decarbonization scenarios are available (see *scenarios* sheet and Section 8.3 of this manual), the scenarios are automatically applied. The indicator in the process inventory is that the linked process starts with "ESTIMATe", e.g., "ESTIMATe electricity" in Figure 5.

4.2.4. Calculation and result presentation

For this calculation and result presentation section of instructions, the numbers in the text refer to Figure 6.

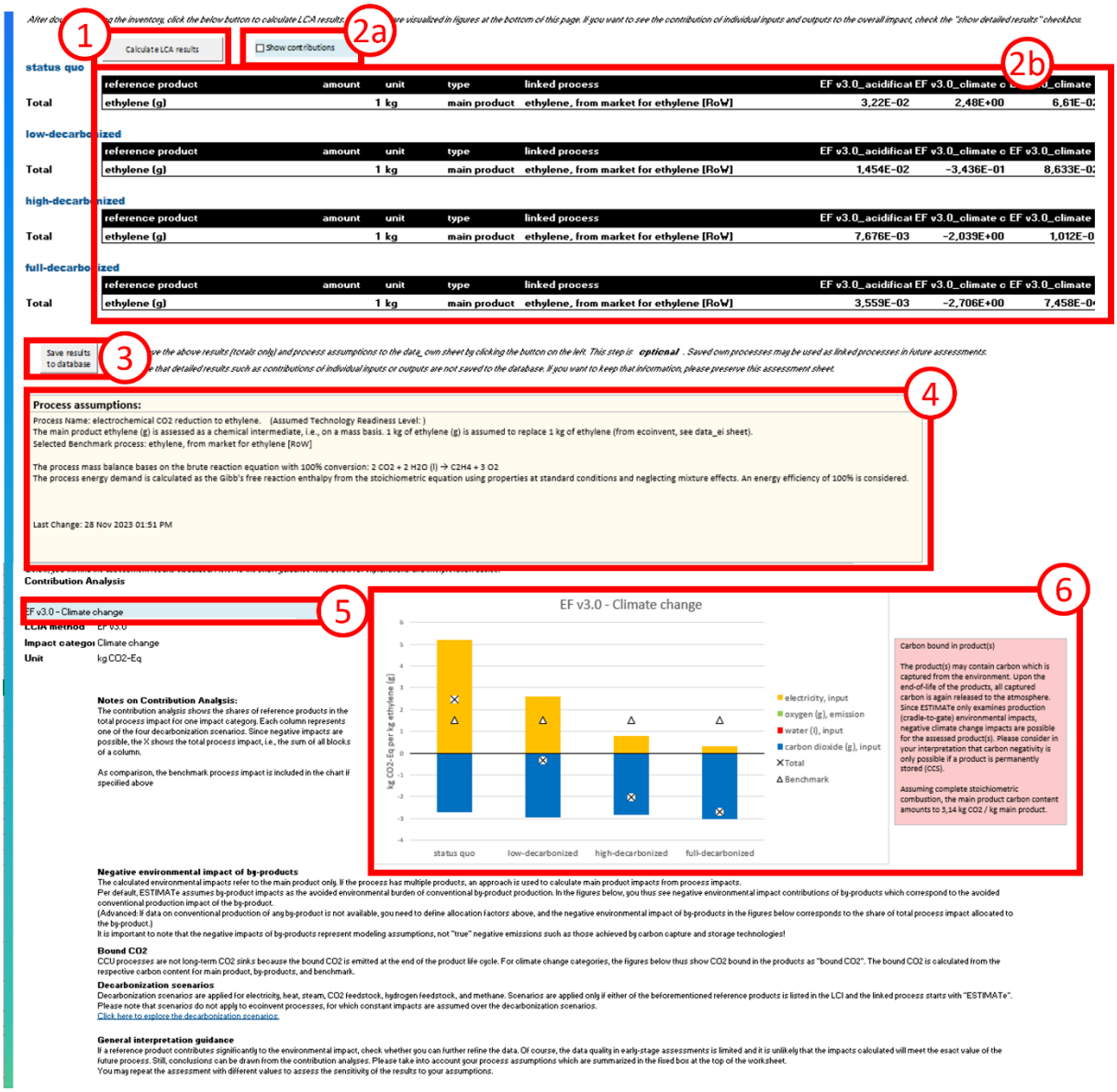


Figure 6: Results section of an exemplary Best-Case Assessment in ESTIMATe

When your process inventory check is finished, click *Calculate LCA results* [1]

The LCA results are calculated for 4 different scenarios (representing levels of decarbonization): status quo, low-decarbonized, high-decarbonized, and full-decarbonized. You will find the numerical results in each scenario below the calculate button [2b] To view the contributions of each process inventory entry to the overall LCA results, click the checkbox *Show contributions* [2]. Otherwise, you see only the overall environmental impacts (column sums).

Optional: Save results to *data_own* sheet [3]

If the LCA results of the studied assessment should be saved to be used as a linked process for further assessments, click the checkbox *Save results to database* [3]. The assessment assumptions and results will be stored on the *data_own* sheet.

Consider the process assumptions section [4] in result interpretation
All assumptions made in your assessment are summarized in the yellow “process assumptions” textbox.

Explore graphical Contribution Analysis results [6] by selecting impact categories from the dropdown menu [5]
You will find explanations and interpretation guidance next to and under the figure and in Section 8 of this manual.

Generate an overview of impact categories (cf. Figure 7)

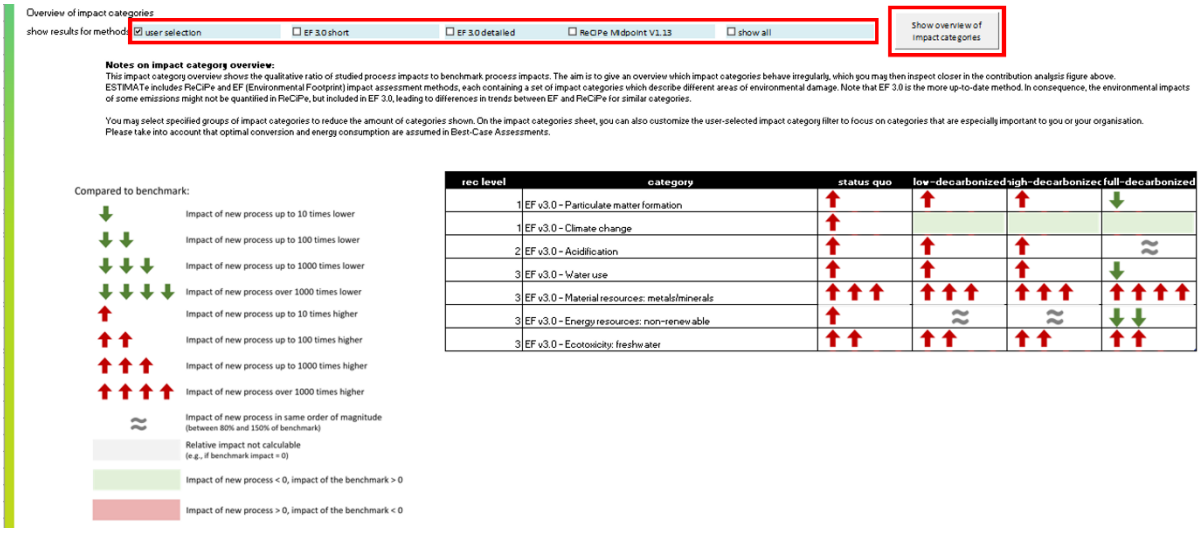


Figure 7: Impact category overview figure of an exemplary Best-Case Assessment in ESTIMATe

- Click the button *Show overview of impact categories* to generate an overview figure of all impact categories
- by checking any check box next to the button, pre-selected sets of impact categories are shown/hidden

The overview figure compares the impact results of the studied assessment with those of the selected benchmark to provide an overview at a glance:

- red arrows mean your assessment has a higher impact than the benchmark process.
- green arrows mean your assessment has a lower impact than the benchmark process.

5. Conducting a Hotspot Assessment

5.1. Introduction: What is a Hotspot assessment?

In Hotspot Assessments, a CCU process is investigated regarding its environmental hotspots and trade-offs. The CCU process is compared either to the current fossil-based benchmark or to a competing CCU route to the same chemical product. Data generation in Hotspot Assessments uses stoichiometric calculations and basic thermodynamics, but users may also input data from external process design software. Data gaps may be filled using estimation methods from the *estimation methods* sheet.

Hotspot assessments allow users to pinpoint the primary contributors to the environmental impact, identifying areas for improving environmental performance, both within the process itself (such as addressing particularly damaging direct emissions) and beyond the process scope (such as the electricity mix). ESTIMATe offers users the flexibility to experiment with the tool, enabling them to gain an understanding of the environmental aspects associated with process design decisions.

5.2. Click instructions

For performing the Hotspot Assessment, you move through the sheet from top to bottom. The following Click Instructions are broken down into four sections: study setup, data generation, data check, and calculation with result presentation.

5.2.1. Study setup: Header of Hotspot Assessment

For this study setup section of instructions, the numbers refer to Figure 8.

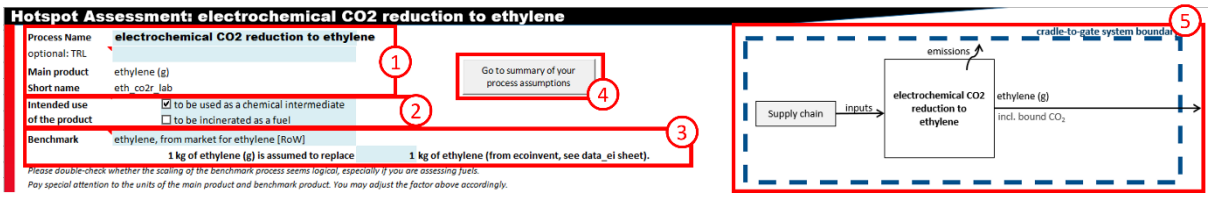


Figure 8: Header of an exemplary Hotspot Assessment in ESTIMATe

Review Assumptions and optionally specify a Technology Readiness Level (TRL) [1]

When creating a new Best-Case Assessment, process name, main product, and short name are directly filled in by the tool. [1] Please do not change the short name or sheet name since otherwise the code will not work anymore. You may, however, change the process name (blue cell). Optionally, you may enter a Technology Readiness Level (TRL). The TRL will be inserted into process assumptions and can help, e.g., in Mitigation Potential Assessments to evaluate technology comparability.

Review the intended use of the product and adapt if necessary [2]

Check the option which applies to your assessment: “to be used as a chemical intermediate” or “to be used as a fuel”. The intended use of the product serves to define the function of a product or process, which is an essential step in LCA. In ESTIMATe, it also determines the unit of the main product: the LCA study is scaled to 1 kg for intermediates, and to 1 MJ energy content for fuels. “To be used as a chemical intermediate” is the default selection when creating an assessment and user may select “to be incinerated as a fuel”.

Review the benchmark process and scaling factor, especially when assessing fuels [3]

- Check whether the selected benchmark product makes sense in your assessment.
- Check whether the scaling factor is sensible, considering the unit of main product and benchmark.
- Repeat these checks whenever you change the intended use of your product!

Background information for step [3]:

The benchmark process impacts will be shown in the result figures to provide context for the CCU assessment results. If available, a default benchmark process is selected from the background database upon sheet creation. Default benchmarks are specified on the *chemicals* sheet. However, you may select any process from *data_ei*, *data_own*, or *scenarios* if it is more applicable to your case.

The scaling factor determines how much of the benchmark product is replaced by the product under study. The scaling factor is set to 1 when a benchmark is automatically set and "to be used as a chemical intermediate" is selected. For fuels, the scaling factor is set using the lower heating value of the assessed main product. Reasoning: most ecoinvent processes have a mass-based unit, e.g., 1 kg of kerosene. The scaling factor thus serves as a conversion factor between the energy content of a fuel product to the mass unit usually used in benchmark processes (using the lower heating value and molar mass of the main product).

Further elements of the header:

Go to summary of process assumptions [4]. At any point in your assessment, you may click the button to get to a summary of your process assumptions located right before the result figures of the assessment (cf. Section 4.2.4)

Overview of assessment system boundaries [5] updates as you make assumptions in ESTIMATe.

5.2.2. Data generation

For this data generation section of instructions, the numbers in the text refer to Figure 9.

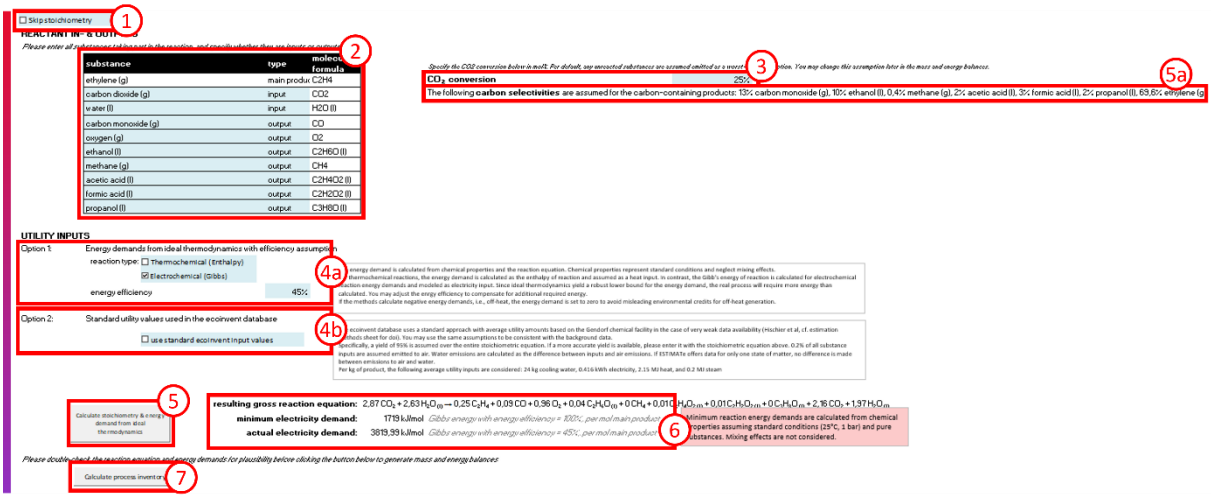


Figure 9: Data generation section of an exemplary Hotspot Assessment in ESTIMATe

Indicate whether data will be generated in ESTIMATe [1]

If you prefer to manually enter process mass and energy in- and output, e.g. from process design software or the literature, you may skip the data generation step by checking the *Skip stoichiometry* checkbox. If you want to skip data generation, proceed to the "data check" section of this manual, Section 5.2.3.

Enter reactants to prepare the gross reaction equation [2]

Select all reactants in the substance column using dropdown menus and define them as inputs or outputs in the type column.

Enter single-pass CO_2 conversion [3]

The CO_2 conversion is considered in the calculation of the brute reaction equation. Substance properties for calculations will be taken from the *chemicals* sheet.

Select an approach to estimate energy demands [4]

Option 1: based on ideal thermodynamics [4a]

Check either the checkbox *thermochemical* or *electrochemical.* The *e*nergy demand will be calculated according to ideal thermodynamics:

- *thermochemical*: reaction enthalpy calculated & assumed as heat input.
- *electrochemical*: Gibb's energy calculated & assumed as electricity input.

You may enter an energy efficiency in relation to the ideal thermodynamic value, which will be considered when calculating the energy demand. If the energy demand is negative, it will be set to zero in the calculate process inventory step to avoid misleading environmental credits for, e.g., off-heat (see step [7]).

Option 2: average values for utility demands [4b]

Alternatively, average utility amounts (electricity, heat, steam, cooling water) and default assumptions may be used. This approach is commonly used in the ecoinvent LCA database if data gaps for chemical processes arise, see Hischier et al.[2] The following assumptions will be made (see info box in ESTIMATe for more detailed information):

- Default values are assumed for electricity, heat, cooling water, and steam input.
- The CO_2 conversion is set to 95% .
- 0,2% of all inputs are assumed directly emitted as fugitives.

Click button to calculate brute reaction equation and energy demand [5]

In the case that your list of substances contains multiple carbon-containing outputs, ESTIMATe will ask you to specify carbon selectivities to each carbon-containing by-product. You must use commas for decimals in the carbon selectivity pop-up! Your assumed carbon selectivities will be entered below the CO_2 conversion value, see [5a] in Figure 9.

Check whether the resulting reaction equation and energy demand look sensible to you [6]

If the results look sensible, proceed. Otherwise, adapt your entries and recalculate ([1] to [5]).

Click button to calculate process inventory, i.e., mass and energy balances [7]

Upon the click, ESTIMATe calculates the "process inventory", i.e., a list of process mass and energy in- and outputs and scales it to the main product unit as specified in the header (cf. "Intended use" in Section 5.2.1). The process inventory is entered into the table below the button.

5.2.3. Data check

For this data check section of instructions, the numbers in the text refer to Figure 10.

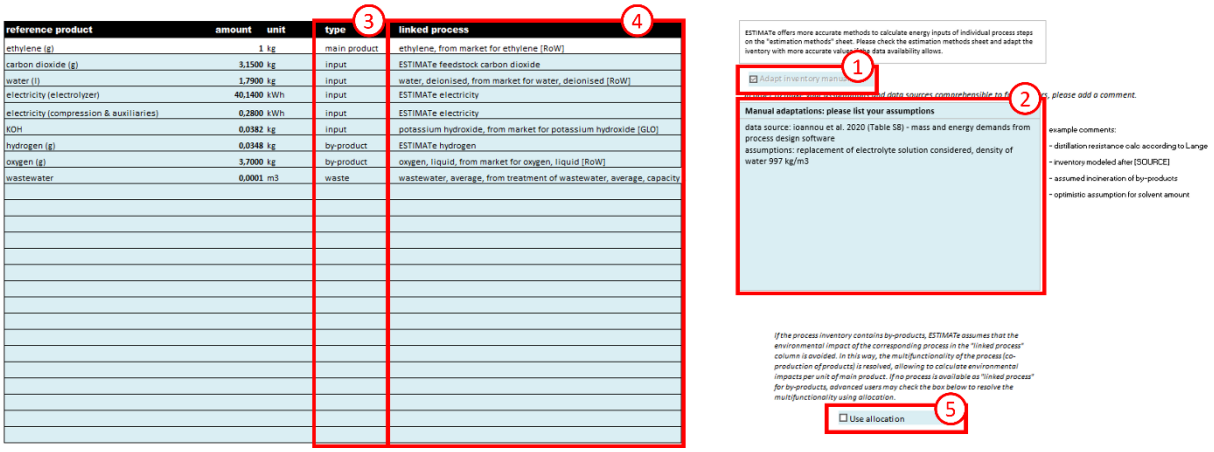


Figure 10: Data check section of an exemplary Hotspot Assessment in ESTIMATe

Before adapting the process inventory, check the "adapt inventory manually" checkbox [1]
Otherwise, you will not be able to adapt anything about your assessment.

Document your adaptations and assumptions in the "manual adaptations" textbox [2]
Documenting your assumptions will help you and future users understand and interpret your assessment results. Your comments will be entered into the process assumptions summary (cf. Section 5.2.4).

Review the type [3] and connected background process [4] for each entry

- Check whether the linked process looks sensible.
- Check the type of your process outputs.

<u>Background information on this step:</u>
If you used stoichiometric methods to calculate the process inventory, the table will already be filled with reference products and their corresponding amount, unit, type and, where available, linked process.

The following types are available: main product (filled in per default), input, by-product, and emission. Per default, all mass outputs assumed as emissions. If a substance would be considered a valuable by-product in a large-scale process, select "by-product" as type instead, and there will be an environmental credit for avoiding production of the by-product in your assessment results. If you have valuable by-products in your assessment, please also refer to the below section "if multiple products exist".

The linked process provides a link to information on environmental impacts of the entry, either in the *chemicals* sheet (for emissions) or the *data_ei, data_own,* or *scenarios* sheets (for inputs, by-products, and wastes). For inputs where decarbonization scenarios are available (see *scenarios* sheet and Section 8.3 of this manual), the scenarios are automatically applied. The indicator in the process inventory is that the linked process starts with "ESTIMATe", e.g., "ESTIMATe electricity" in Figure 5.

Add products to the process inventory
This step is optional if you used stoichiometry to generate data, and mandatory if you skipped the stoichiometry in the data generation section. You may use estimation methods included in ESTIMATe as data source, see Section 6 - Spotlight: Using estimation methods in Hotspot Assessments.

After checking the *Adapt inventory manually* checkbox [1], the process inventory can be adjusted manually, i.e., you may add or delete reference products and their corresponding amount, unit, type and linked process.

Guidance for adding lines to the process inventory:

- In each line, all cells are mandatory, i.e., each line needs a reference product, amount, unit, type, and linked process.
- Types
    - All inputs to the process are "inputs"
    - For outputs distinguish between:
        - "emissions" – substances that are directly emitted to the environment
        - "by-products" – substances that are considered valuable and possible to sell/replace conventional production (also refer to the "If multiple products exist" section below)
        - "wastes" – substances that go to waste treatment processes, such as contaminated wastewater.
- Linked process for chemical emissions
    - For emissions, "characterization factors" in the *chemicals* sheet indicate the environmental impacts resulting from their emission.
    - If a chemical adheres to the naming convention, is defined as an emission in the process inventory, and its characterization factors are defined in the *chemicals* sheet, the reference product name is filled in to the linked process column to signify the emission was found. If there are no characterization factors in *chemicals*, the environmental impact of the emission cannot be considered in the calculation. This is indicated by "[not characterized]" in the linked process cell, and user guidance will be provided in the process assumptions block (cf. Section 5.2.4).
    - Naming convention for chemicals: [trivial name] ([state of matter]), e.g., "hydrogen (g)".
- Linked process for other types
    - You may choose the linked processes from the dropdown menu, which includes all processes from the sheets *data_ei*, *data_own*, and *scenarios*. There is the option to filter the dropdown by typing into the linked process cell. If the dropdown or filter does not work, select a different cell before reselecting the cell with the malfunctioning dropdown. Alternatively, you can look directly into the sheets *data_ei*, *data_own*, and *scenarios* and copy the process name from the column named "search column".
    - If you have the option to choose an "ESTIMATe" process for your reference product, you should do so, except if you have a good reason not to. Decarbonization scenarios are automatically applied to "ESTIMATe" processes. This refers specifically to the following reference products:
        - feedstock carbon dioxide (naming convention: "carbon dioxide (g)"),
        - hydrogen (naming convention: "hydrogen (g)",
        - electricity,
        - heat,
        - steam,
        - methane/natural gas (naming convention: "methane (g)")
    - If you adhere to naming conventions in the reference product column (mind to not have, e.g., additional spaces!), linked processes will be filled in automatically after type specification in the following cases:

- Chemicals from the *chemicals* sheet, naming convention [trivial name] ([state of matter]), e.g., “hydrogen (g)”.
    - If the chemical is defined as an input or by-product, the linked background database process as specified on the *chemicals* sheet is filled in.
    - If the chemical is defined as an emission and characterization factors are defined in the *chemicals* sheet, the reference product is filled in to signify the emission was found. If there are no characterization factors in *chemicals*, the environmental impact of the emission cannot be considered in the calculation. This is indicated by “[not characterized]” in the linked process cell.
  - For the following utilities linked processes are filled in (for input and by-product types), if naming conventions are followed: “electricity”, “heat”, “steam”, “cooling water”
- Units
  - Emissions are always assumed in kg
  - Units of flows of other types than emissions need to correspond to the unit of the linked process. Typical units for ecoinvent processes are: kg, MJ, kWh, m3, unit
  - You will be alerted of inconsistent units upon calculation.

If multiple products exist

Option 1 (default): avoided burden

If reaction outputs are declared as *by-products*, they receive an environmental impact credit for avoiding conventional production. This option will take place by default if by-products exist in the process inventory of the assessment and the checkbox *Use allocation* [5] is not checked. For the avoided burden to work, each by-product needs to have a valid linked process specified in the “linked process” column of the process inventory.

Option 2 (recommended to advanced users only): use allocation [5]

If an avoided burden approach is not possible, or if more experienced LCA practitioners want to check the sensitivity of results towards the allocation method, allocation by a criterion may be employed. To do so, check the “*use allocation*” checkbox, and an allocation table will appear under the process inventory table (cf. Figure 11). (Note that the checkbox only appears if at least one by-product is specified in the process inventory.

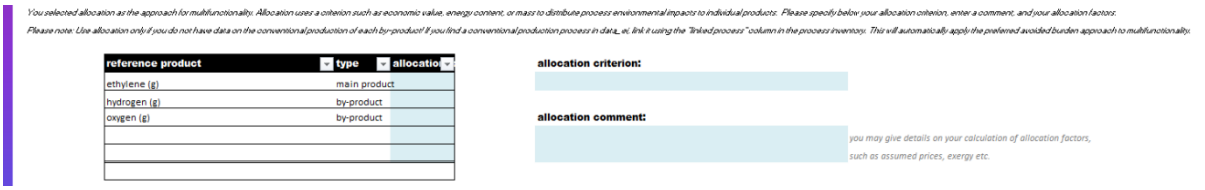


Figure 11: Allocation section on an exemplary Hotspot Assessment sheet. (Located directly under the process inventory)

In the allocation table (cf. Figure 11),

- All co-products are already filled in automatically. (A maximum of 5 co-products is supported for the allocation calculation).
- Specify an allocation criterion (we recommend the economic value).
- For each reference product, specify the allocation factor, i.e., the share of total environmental impact allocated to the product. The sum of all allocation factors must be 1.
- Add information on the allocation assumptions in the area of *allocation comment* (e.g., assumed prices, sources, reasoning for choosing criterion).

5.2.4. Calculation and result presentation

For this calculation and result presentation section of instructions, the numbers in the text refer to Figure 12.

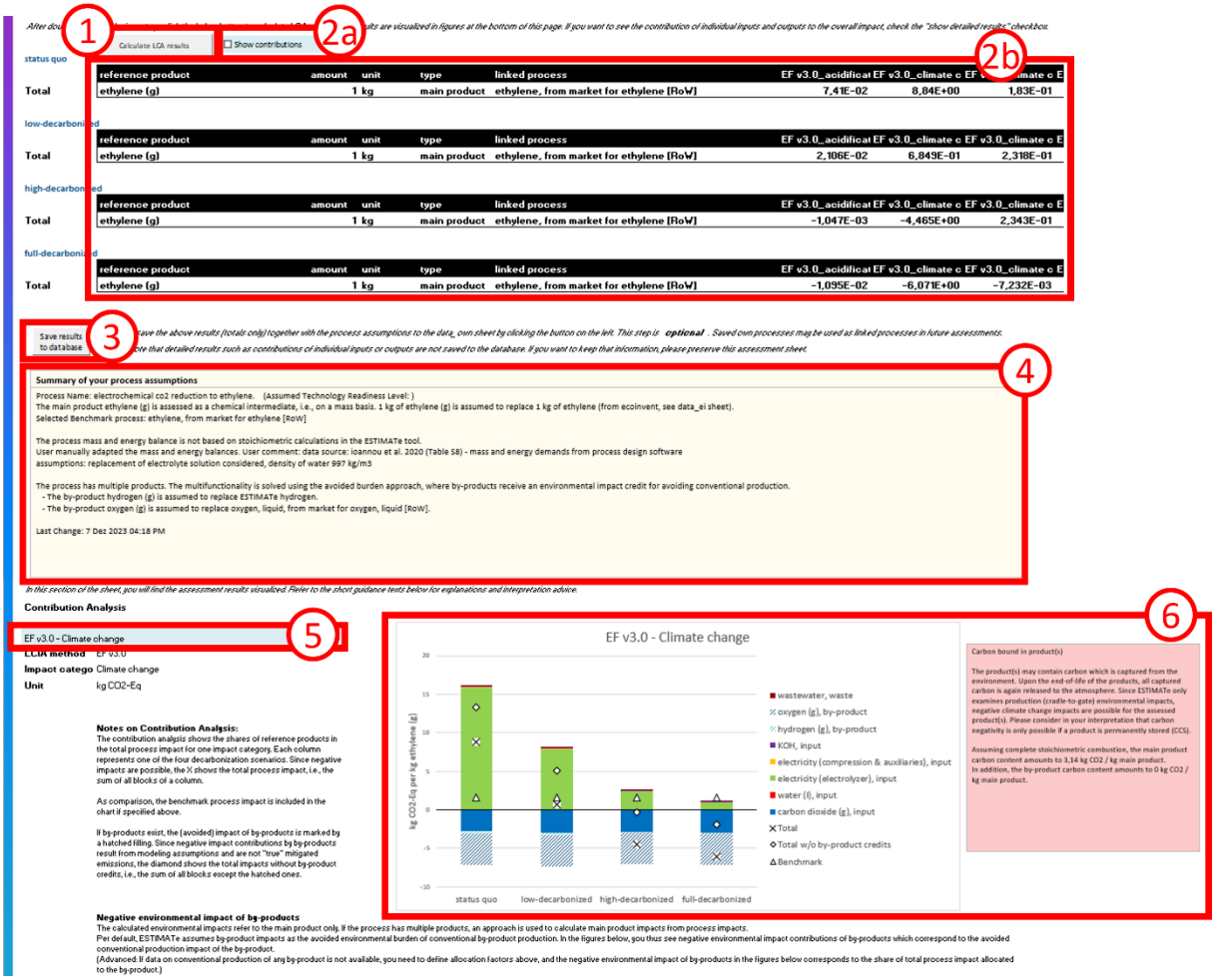


Figure 12: Results section of an exemplary Hotspot Assessment in ESTIMATe

When you are satisfied with your process inventory, click *Calculate LCA results* [1]

The LCA results are calculated for 4 different scenarios (representing levels of decarbonization): status quo, low-decarbonized, high-decarbonized, and full-decarbonized. You will find the numerical results in each scenario below the calculate button [2b] To view the contributions of each process inventory entry to the overall LCA results, click the checkbox *Show contributions* [2]. Otherwise, you see only the overall environmental impacts (column sums).

Optional: Save results to data_own sheet [3]

If the LCA results of the studied assessment should be saved to be used as a linked process for further assessments, click the checkbox *Save results to database* [3]. The assessment assumptions and results will be stored on the *data_own* sheet.

Consider the process assumptions section [4] in result interpretation

All assumptions made in your assessment are summarized in the yellow “process assumptions” textbox.

Explore graphical Contribution Analysis results [6] by selecting impact categories from the dropdown menu [5]

You will find explanations and interpretation guidance next to and under the figure and in Section 8 of this manual.

Generate an overview of impact categories (cf. Figure 13)

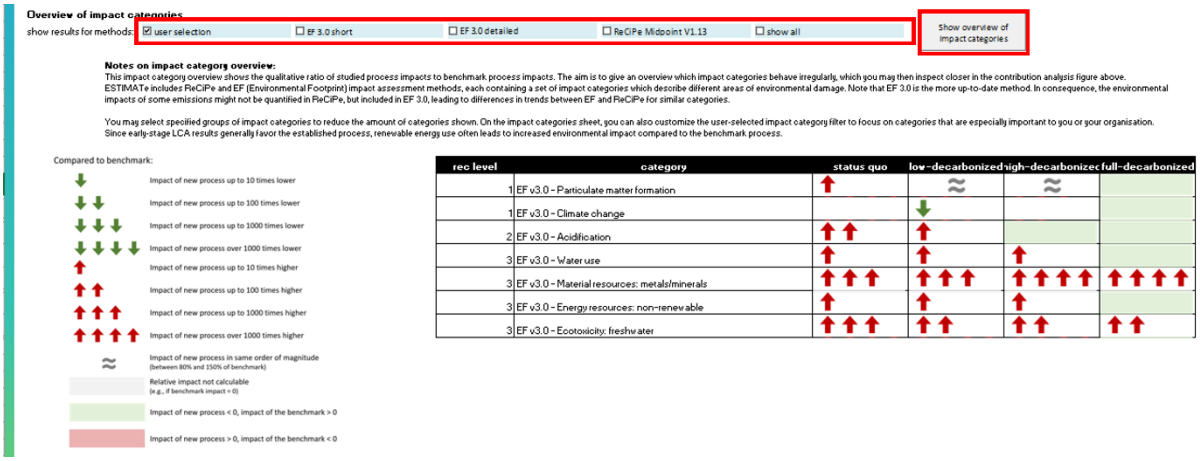


Figure 13: Impact category overview figure of an exemplary Hotspot Assessment in ESTIMATe

- Click the button *Show overview of impact categories* to generate an overview figure of all impact categories
- by checking any check box next to the button, pre-selected sets of impact categories are shown/hidden

The overview figure compares the impact results of the studied assessment with those of the selected benchmark to provide an overview at a glance:

- red arrows mean your assessment has a higher impact than the benchmark process.
- green arrows mean your assessment has a lower impact than the benchmark process.

6. Spotlight: Using estimation methods in Hotspot Assessments

Life Cycle Assessment studies generally require detailed mass and energy balances of the studied process (ISO 14044:2006; ISO 14040:2006). In early stages of process development, however, comprehensive data of the industrial size process are not available. Consequently, suitable estimation methods are required to fill data gaps. Since the data availability increases along with the process development, the CCU guidelines (Langhorst et al. 2022) recommend methods to close data gaps depending on the Technology Readiness Level.

Estimation methods recommended up to TRL 2 are mostly stoichiometry-based and heuristic approaches. In ESTIMATe, these estimation methods are directly included in the Best-Case Assessment and Hotspot Assessment sheets, and their results scaled to the functional unit.

At TRL 3 and 4, estimation methods are based on simple process design equations for individual equipment, such as distillation columns or dryers. The calculation of mass and energy balances of the overall process from individual equipment necessitates a basic flowsheet of the process, which ESTIMATe does not provide. Instead, the *estimation methods* sheet provides the guideline-recommended process design equations for TRL 3 and 4.

This section briefly introduces the structure of the *estimation methods* sheet and provides an example of applying an estimation method for determining a separation energy demand.

6.1. The estimation methods sheet

The sheet begins with a short explanation of the purpose of estimation methods in ESTIMATe. A short overview of two non-automatable methods for direct environmental impact and fugitive emissions estimation follows, including a link to the literature source for each method.

For the automated energy demand estimation methods, an interactive table provides an overview of applicable methods (cf. Figure 14). In the overview table, select the data currently available to you in the leftmost column [1]. The rows corresponding to selected data [2] turn green to indicate data availability. For each method, a button [3] provides a shortcut to the method's location on the estimation method sheet. As soon as all data for a method are available, the button turns green.

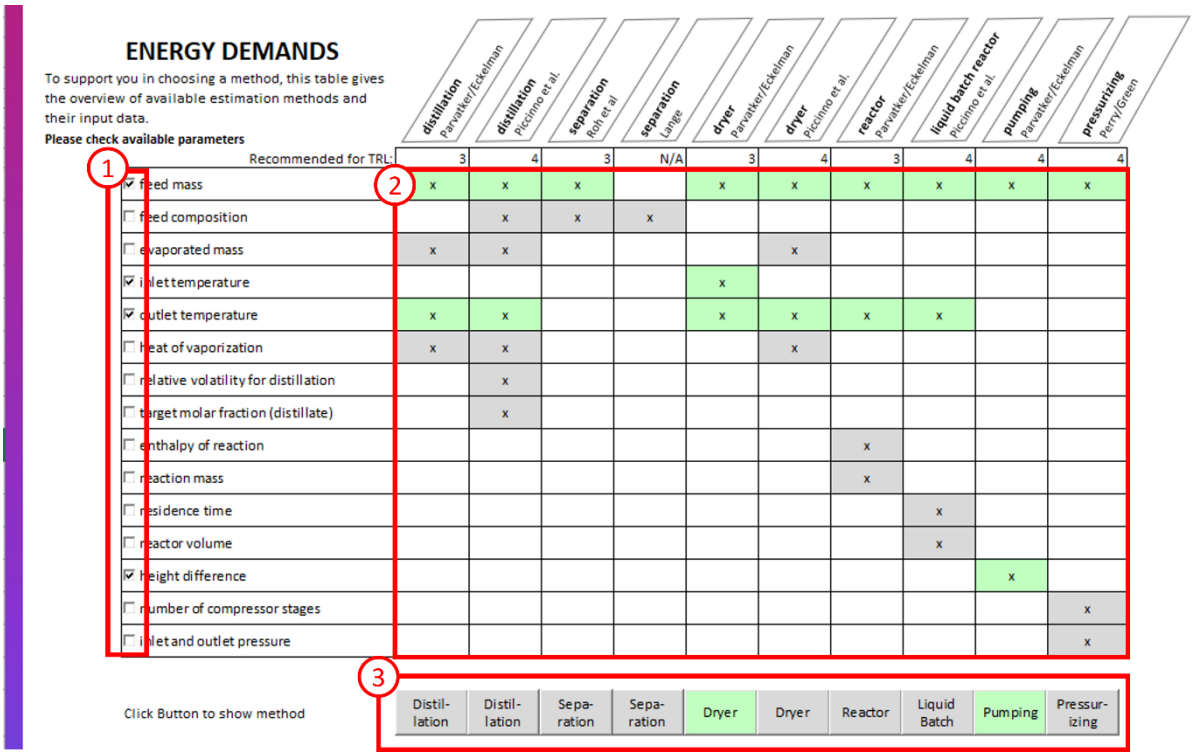


Figure 14: Overview table of estimation methods for energy demands

Below the overview table, energy demand estimation methods are listed. The information provided for each method is structured as shown in Figure 15. For each method, ESTIMATe offers a method description, underlying equations, and an "assumptions and limitations" section. Method name, recommended TRL according to the CCU guidelines, and a link to the primary literature source are included. Input data is distinguished into mandatory input data, which are necessary for the calculation to execute, and optional input data for which default values are used if the user does not specify values. Each method further has a parameter information "(i)" and a "Calculate" button.

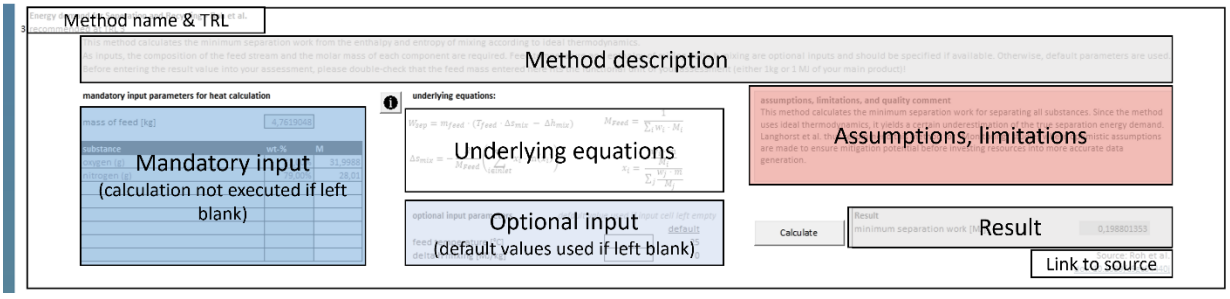


Figure 15: Structure of an energy demand estimation method

6.2. Example: separation energy demand estimation for CO_2 recycle

In an exemplary Hotspot Assessment for electrochemical CO_2 reduction to ethylene, stoichiometry was used to generate data. Due to low CO_2 conversion, the calculated process inventory (cf. Figure 16) includes around 13.5 kg of CO_2 emissions and 18 kg CO_2 feedstock input per kg of ethylene produced. Consequently, the user wants to implement a recycle of unreacted CO_2.

reference product	amount	unit	type	linked process
ethylene (g)	**1,00**	kg	main product	ethylene, from market for ethylene [RoW]
carbon dioxide (g)	**18,03**	kg	input	ESTIMATe feedstock carbon dioxide
water (l)	**6,76**	kg	input	water, deionised, from market for water, deionised [RoW]
carbon dioxide (g)	**13,52**	kg	emission	carbon dioxide (g)
water (l)	**4,71**	kg	emission	water (l)
carbon monoxide (g)	**0,37**	kg	emission	carbon monoxide (g)
oxygen (g)	**4,71**	kg	emission	oxygen (g)
ethanol (l)	**0,24**	kg	emission	ethanol (l)
methane (g)	**0,01**	kg	emission	methane (g)
acetic acid (l)	**0,06**	kg	emission	acetic acid (l)
formic acid (l)	**0,09**	kg	emission	formic acid (l)
propanol (l)	**0,04**	kg	emission	propanol (l)
electricity	**37,82**	kWh	input	ESTIMATe electricity
hydrogen (g)	**0,04**	kg	emission	hydrogen (g)

Figure 16: Exemplary process inventory of CO_2 reduction to ethylene, generated in ESTIMATe

After selecting “adapt inventory manually” to allow for adaptions to the process inventory, the user adjusts the values of carbon dioxide input and emission, subtracting the amount of recycled carbon dioxide from both values. They might decide to account for purge of CO_2 in the recycle. Assuming a purge of 0.15 kg CO_2, 13.35 kg of CO_2 are successfully recycled, lowering the CO_2 input to 4.65 kg, and the CO_2 emission to the 0.15 kg lost in the recycle.

Next, the user employs an estimation method for the separation energy required for the recycle. Adding a new line to the process inventory (cf. Figure 17), they specify the reference product, for instance as “minimum separation energy demand for recycle” with the type “input”. The user selects the energy demand to be supplied by electricity by choosing “ESTIMATe electricity” as the linked process.

minimum separation electricity for recycle	**2,2500**	kWh	input	ESTIMATe electricity

Figure 17: Line added to the process inventory for the separation energy demand. Amount determined using estimation method.

To determine the amount of electricity required for the separation, the user uses the estimation method for separation and recycling by Roh et al.[3] which is the third method on the *estimation methods* sheet. All mandatory inputs can be obtained from the inventory in Figure 16. The inputs into the estimation method are depicted in Figure 18 and include a list of all gaseous products. The user further enters the sum of the weights of all gaseous products as “mass of feed” and specifies the composition in weight percents. Clicking “Calculate”, the minimum energy demand for separation is calculated to $0.625\ MJ$. The user may now copy the calculated amount and unit and enter them into the line added in the Hotspot Assessment (Figure 17). A unit conversion might be necessary if energy is supplied in the form of electricity, in this case: $0.625\ MJ\ = 2.25\ kWh$. If applicable, ESTIMATe will alert the user of unit inconsistencies when calculating the Hotspot Assessment but not directly upon entering the amount into the process inventory.

Energy demand for Seperation and Recycling - Roh et al.

3 recommended at TRL 3

This method calculates the minimum separation work from the entha
As inputs, the composition of the feed stream and the molar mass of
Before entering the result value into your assessment, please double

mandatory input parameters for calculation

mass of feed [kg]	15,114

substance	wt-%	M
ethylene (g)	6,6%	28,0532
carbon monoxide (g)	2,5%	28,0101
hydrogen (g)	0,3%	2,01588
methane (g)	0,0%	16,0425
carbon dioxide (g)	90,6%	44,0095

Figure 18: Cutout of the estimation method used for separation energy demand estimation

For future reference, any assumptions and used estimation methods should be listed on the Hotspot Assessment sheet in the “Manual adaptations” textbox. The final process inventory and manual adaptations textbox are shown in Figure 19.

reference product	amount	unit	type	linked process
ethylene (g)	1,00	kg	main product	ethylene, from market for ethylene [RoW]
carbon dioxide (g)	4,65	kg	input	ESTIMATe feedstock carbon dioxide
carbon dioxide (g)	0,15	kg	emission	carbon dioxide (g)
water (l)	6,76	kg	input	water, deionised, from market for water, deionised [RoW]
water (l)	4,71	kg	emission	water (l)
carbon monoxide (g)	0,37	kg	emission	carbon monoxide (g)
oxygen (g)	4,71	kg	emission	oxygen (g)
ethanol (l)	0,24	kg	emission	ethanol (l)
methane (g)	0,01	kg	emission	methane (g)
acetic acid (l)	0,06	kg	emission	acetic acid (l)
formic acid (l)	0,09	kg	emission	formic acid (l)
propanol (l)	0,04	kg	emission	propanol (l)
electricity	37,82	kWh	input	ESTIMATe electricity
minimum separation electricity for recycle	2,25	kWh	input	ESTIMATe electricity
hydrogen (g)	0,04	kg	emission	hydrogen (g)

☑ Adapt inventory manually

In order to make your assumptions and data sources comprehensible to future users, please add a comment.

Manual adaptations: please list your assumptions

inventory represents expertimental data from li et al. which was also used for the lab-scale assessment in khoo et al.

separation electricity calculated as minimum separation work from estimation method 3
--> co2 recycle modeled by adding separation energy demand and reducing co2 input value by recycled value.
0.15kg of co2 assumed as recycling loss (generous 1% of recycled mass)

Figure 19: Final process inventory and exemplary manual adaptations comment

7. Conducting a Mitigation Potential Assessment

7.1. Introduction: What is a Mitigation Potential Assessment?

Mitigation Potential Assessments (MPA) enable the direct comparison of environmental impacts mitigated by two CCU processes. For this purpose, ESTIMATe assumes that the CCU processes replace the conventional production ("benchmark") of their respective product, cf. Figure 20. The processes to be compared need to be modeled as Hotspot Assessment in ESTIMATe beforehand.

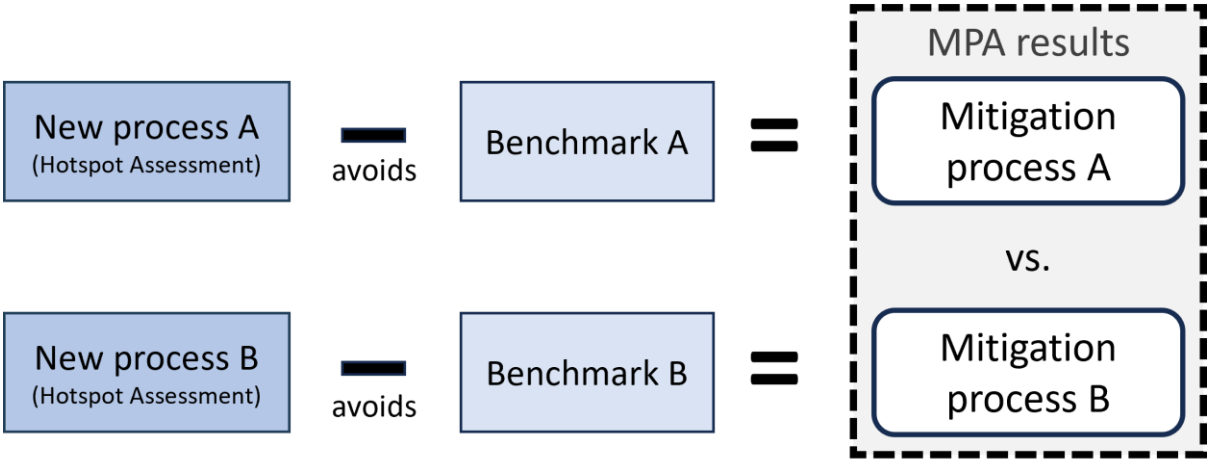


Figure 20: Schematic of MPA studies in ESTIMATe. MPA studies compare the mitigation of two process options. The mitigation of each option is determined by subtracting the benchmark process environmental impacts from the environmental impacts of the new process.

To ensure meaningful results, MPA studies must compare the two processes on a fair basis of comparison, for which two cases exist:

1. **Comparison of processes with the same main product:**

   If the compared processes yield the same main product, the comparison takes place on the basis of one unit of main product, e.g., 1 kg of ethylene.

2. **Comparison of processes with different main products:**

   In the case of different main products, the comparison of the mitigation achieved by each process per unit of main product would not be fair since the main products fulfill different functions. For instance, comparing 1kg of ethylene to 1kg of methanol would be an "apples to oranges" comparison. Instead, the comparison in such MPA studies takes place based on a shared renewable resource. An MPA study on processes with differing main products answers the question "Given 1 unit of shared resource, which process achieves higher environmental impact mitigation?". In this way, MPA studies support decision-making under limited resource availability.

7.2. Click Instructions

7.2.1. Study setup

To perform an MPA study in ESTIMATe, use the *New Assessment* sheet to create an empty MPA sheet. The following steps are required on the MPA sheet (cf. Figure 21):

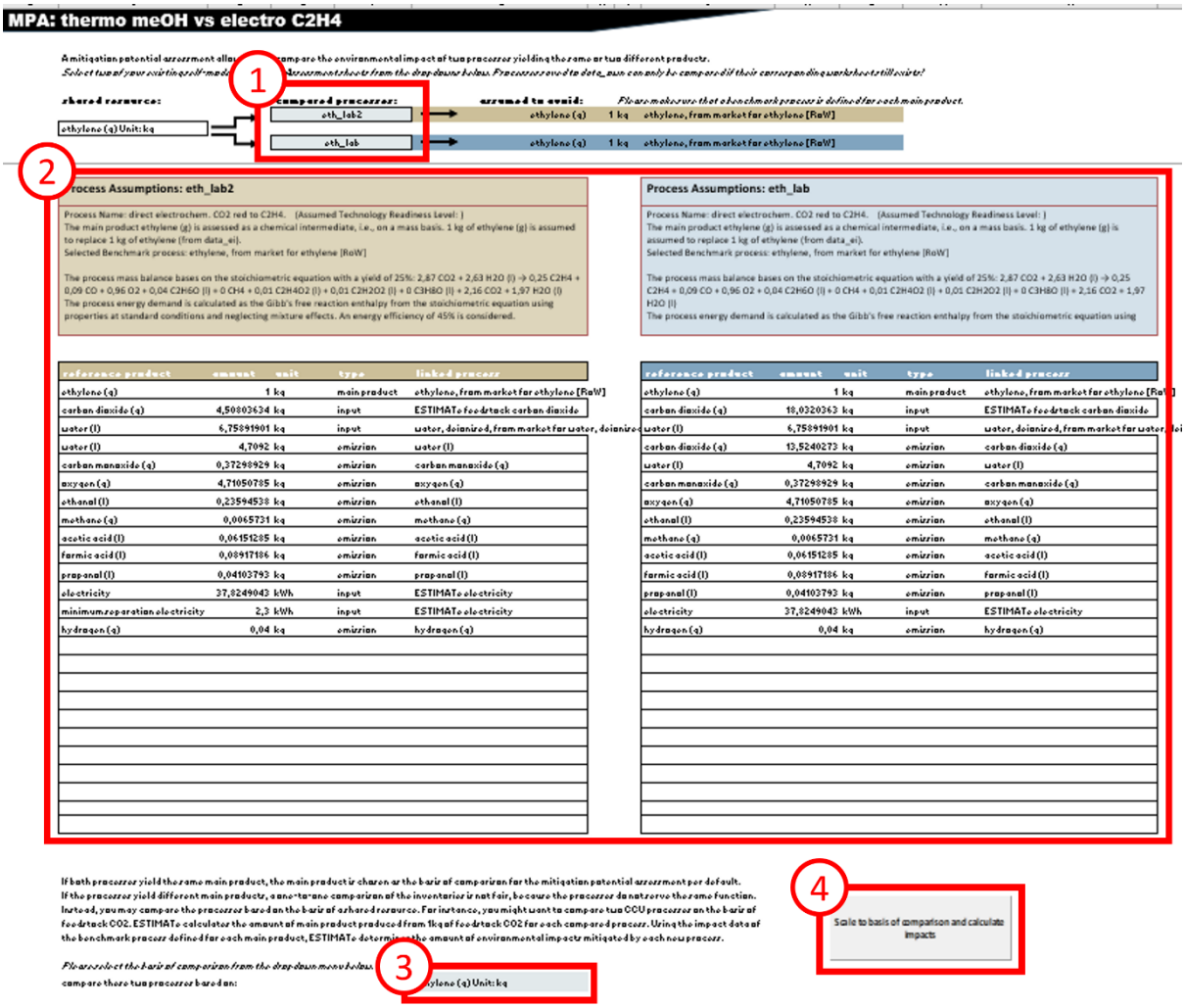


Figure 21: Calculation steps on an exemplary Mitigation Potential Assessment sheet in ESTIMATe

Select the processes to compare in the MPA header [1]

Please select the processes you want to compare from the dropdown menus [1]. Since MPAs are intended to compare Hotspot Assessments, the dropdown menu comprises all Hotspot Assessment sheets currently in the ESTIMATe tool.

Please note: the processes on the MPA sheet are not updated automatically when opening the sheet. If you have made changes to the Hotspot Assessment to be compared in your MPA. Re-select the Hotspot Assessment from the dropdown menu in the MPA header. The process will then be updated on the MPA sheet.

Check the copied process inventories [2]

After choosing a process in the header, the process assumptions, inventory, and results are copied to the MPA sheet. Please double-check if you selected the intended process.

Select the shared resource [3]

Select a basis of comparison. If the compared processes yield the same main product, the main product is selected as basis of comparison by default. In the case of non-identical main products, chose a shared resource as basis of comparison from the dropdown menu. For CCU processes, sensible bases of comparison might be feedstock CO_2 or renewable electricity. The selection of different shared resources is recommended to users with LCA expertise since it might influence the study interpretation.

Start the calculation [4]
A click on the button "scale to basis of comparison and calculate impacts" scales both process inventories to the shared resource, calculates the LCA results and creates the contribution analysis figure.

7.2.2. Result presentation

You successfully completed the MPA calculation. The calculation results are now displayed below the resource selection (cf. Figure 22).

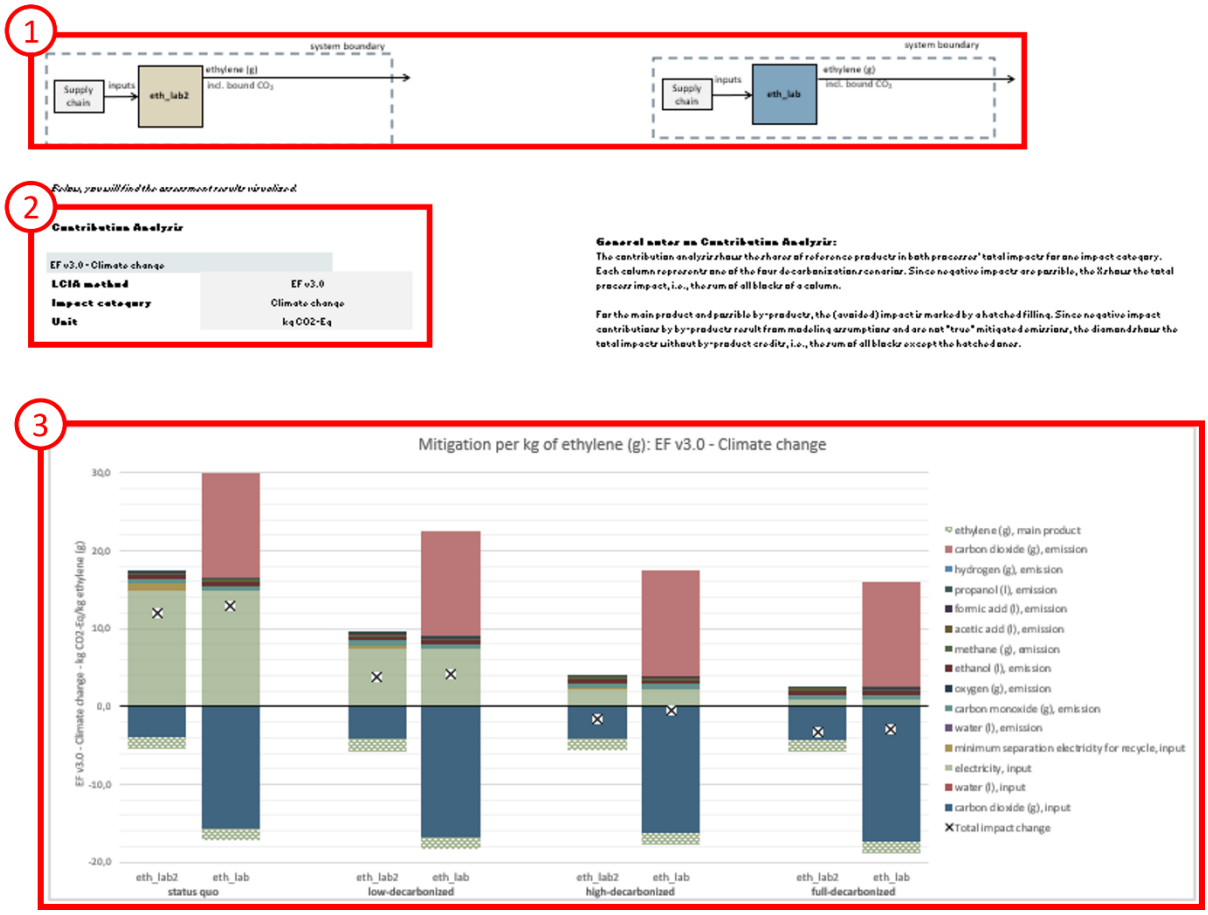


Figure 22: Exemplary Mitigation Potential Assessment sheet result section part 1: overview of system boundaries and contribution analysis chart

Refer to the system boundary charts [1]
The system boundary chart for each process illustrates where in the process the basis of comparison occurs: as the main product, as an input, or a by-product? Furthermore, it indicates whether the process produces any by-products. You may refer to this simplified visual representation of the process during interpretation.

Select an impact category for the contribution analysis [2]

From the dropdown menu, select the impact category you are interested in. The contribution analysis chart is updated accordingly.

Find the visualized results in the contribution analysis chart [3]
The chart displays the environmental impacts of both processes through the decarbonization scenarios in the selected impact category. Assumed credits for avoiding conventional production of main products and possible by-products are hatched to clearly distinguish assumed credits from the other contributors to the environmental impact. Per bar, a total and a total without by-product credits is marked. To the right of the chart, a table contains numerical results.

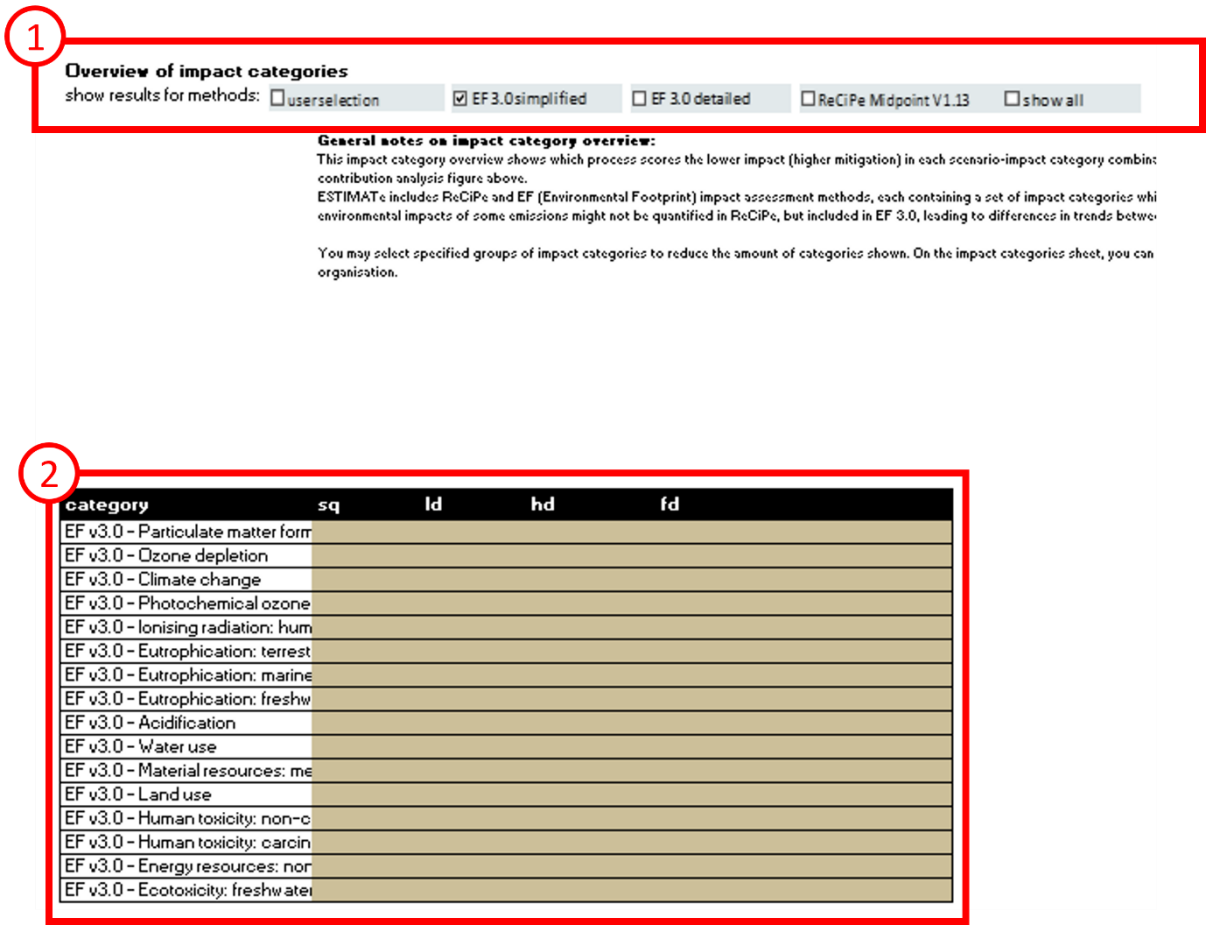


Figure 23: Exemplary Mitigation Potential Assessment sheet result section part 2: overview of all impact categories

Finally, an overview figure (cf. Figure 23) summarizes results in all impact categories briefly.

Select an impact category set [1]
Since ESTIMATe includes many impact categories, a shortened overview can be desirable. The checkboxes provide pre-selected sets of impact categories. Per default, all impact categories are shown.

Find the result overview in the overview table [2]
In, the overview of all impact categories, the color indicates which process has a lower impact in a given impact category and scenario. In contrast to the contribution analysis figure, no detailed information is shown for the processes. The overview figure is a raw comparison of the absolute values *including by-product credits.*

8. Interpreting ESTIMATe results

8.1. General interpretation guidance

Negative impacts in Best-Case and Hotspot Assessments

There are two possible reasons for negative environmental impacts:

a) Negative impacts due to by-product credit assumptions
   If by-products occur in the assessed process, ESTIMATe gives an environmental credit for the replacement of the conventional production of the by-products. Such assumptions are widely used in LCA studies to calculate main product-specific environmental impacts in multi-functional processes. In all impact categories, by-product credits can exceed process impacts, leading to negative overall process impacts. Negative impacts resulting from such assumptions on avoided environmental burden are methodologic assumptions and do not represent true removal of, e.g., carbon dioxide, from the atmosphere.
b) Negative Global Warming Impact due to carbon stored in product
   Due to the "cradle-to-gate" system boundaries of LCA studies in ESTIMATe, negative Global Warming Impacts (GWI) can be reached. Specifically, carbon captured from the environment may still be present in the product at the end of the assessment scope but will be emitted to the atmosphere at the product's end of life. Only technologies achieving permanent CO_2 storage may achieve true carbon negativity. To avoid misinterpretation of negative total impacts as "negative emission technologies", ESTIMATe specifies the amount of CO_2 bound in the product at the end of the assessed study scope in a text box next to GWI contribution analyses.

Recommendation levels for impact categories

ESTIMATe uses literature methods for Life Cycle Impact Assessment. Specifically, the ReCiPe Midpoint V1.14 and Environmental Footprint EF3.0 methods are implemented. Not all impact assessment methods are equally certain. For instance, toxicity impacts are more difficult to characterize than ozone depletion impact. Thus, EF3.0 impact categories include a classification of the uncertainty of the impact category, i.e., a "level of recommendation". The higher the level of recommendation, the more uncertain the impact category. Levels of recommendation for EF3.0 methods are included in ESTIMATe, both in result overview tables and on the *impact categories* sheet.

Impact categories other than climate change

ESTIMATe calculates cradle-to-gate environmental impacts across various environmental impact categories and offers benchmark data where possible, potentially revealing trade-offs between impact categories. However, ESTIMATe does not rate the severity of these trade-offs or define acceptable impact increases. Companies and users are encouraged to establish their own No-Go criteria for impact categories based on their sustainability goals, in addition to the No-Go criterion related to unachievable climate change impact mitigation.

Bias in favor of established technology

Conventional chemical processes have been optimized for decades in terms of efficiency and utility consumption. Consequently, there is a general bias in LCA studies in favor of the established technologies. When interpreting results, take this bias into account especially for non-GWI impact categories.

Constant environmental impacts of ecoinvent processes through decarbonization scenarios

For ecoinvent processes, the environmental impacts are assumed constant throughout the decarbonization scenarios. This means that factors related to background system changes, including

alterations in the electricity grid mix, are not considered within the scope of ESTIMATe for ecoinvent processes. While changes in impact are anticipated for ecoinvent processes similar to scenario processes, these changes are expected to be of a smaller magnitude because of the higher relative importance of scenario inputs for CCU process than for conventional processes. For instance, direct emissions in conventional processes would not be affected by background system scenarios.

8.2. Interpretation of MPA studies

In addition to the above-mentioned interpretation guidance, some methodologic particularities apply to Mitigation Potential Assessment studies, which compare two CCU processes modeled in ESTIMATe. For a fair comparison of two Life-Cycle Assessment studies, the compared processes need to fulfill the same function. The following distinction needs to be made to allow for a fair comparison of the processes in ESTIMATe:

- For *processes yielding the same main product*, the main product is selected as the basis of comparison. The question answered is "Which process achieves higher impact mitigation compared to the benchmark process?"
- Since *processes yielding different main products* cannot be compared 1:1, a basis of comparison needs to be defined. Usually, the user selects a resource shared by both processes as the basis of comparison. The question answered by the assessment then changes to "per unit of shared resource used, which process achieves higher impact mitigation?". This question reflects that resources necessary for CCU processes are often scarce, e.g., captured CO_2 or renewable electricity. For CCU processes, a comparison based on the mass of feedstock CO_2 is recommended. A comparison based on renewable electricity use makes sense if electricity is the main form of energy consumed by the process.
    - When selecting a basis of comparison, make sure that the selection makes sense for your process context. For instance, when comparing an electrochemical process with high electricity demand to a thermochemical process with high heat demand and low electricity demand, a comparison based on electricity would be possible, but probably unfair.
    - Furthermore, inspect your process inventory closely after pressing the "scale to basis of comparison" button to make sure the scaling to the basis of comparison has taken place as you envisioned. As further support, the "system boundary" figures below the process inventory display in bold font where in your process inventory the selected basis of comparison was found and considered for scaling. (cf. Figure 24, where two processes are scaled to the amount of feedstock CO_2 used in them)

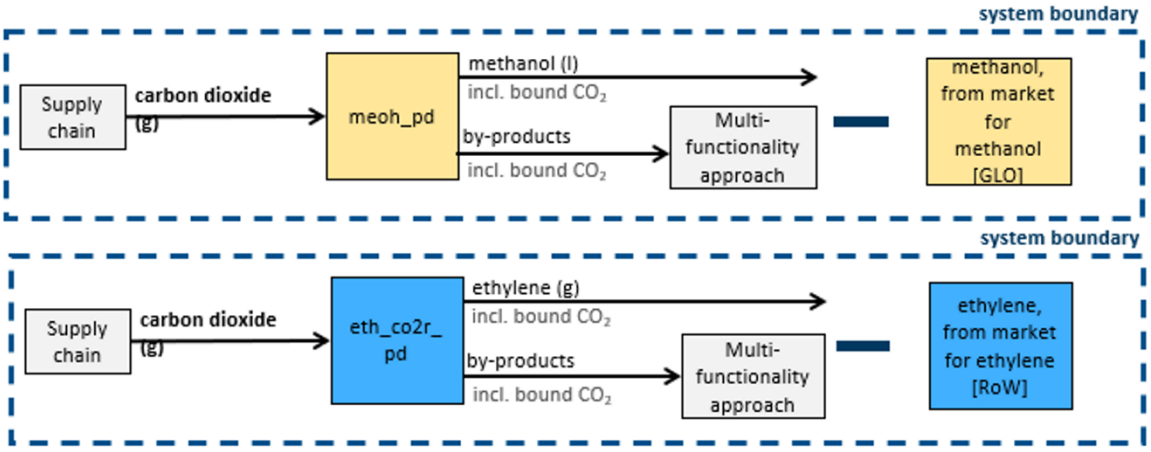


Figure 24: Example for system boundary figure in Mitigation Potential Assessments in ESTIMATe. Two processes producing different main products (methanol and ethylene, respectively) are scaled to a common shared resource: feedstock carbon dioxide, indicated by the bold font.

In MPA studies, the main product is assumed to avoid the benchmark technology and thus receives an "environmental credit". This procedure is similar to that of by-product credits which is explained in the Section "General interpretation guidance". In the contribution analysis figure (cf.

Figure 25), main product credits are hatched differently than by-product credits to allow their distinction. Main product credits are always included in totals. Due to the main product credits, the **totals in the contribution analysis figure in MPA studies show mitigated environmental impact** instead of absolute environmental impact per kg of main product. Consequently, only processes with negative total values achieve impact mitigation. Positive total values indicate a higher impact for the new process compared to the benchmark process. Please note that the environmental impact credit awarded to main products represents the selected benchmark process. In particular, ecoinvent processes give a momentary snapshot of the status quo environmental impacts and do not consider background system or technology changes in the future.

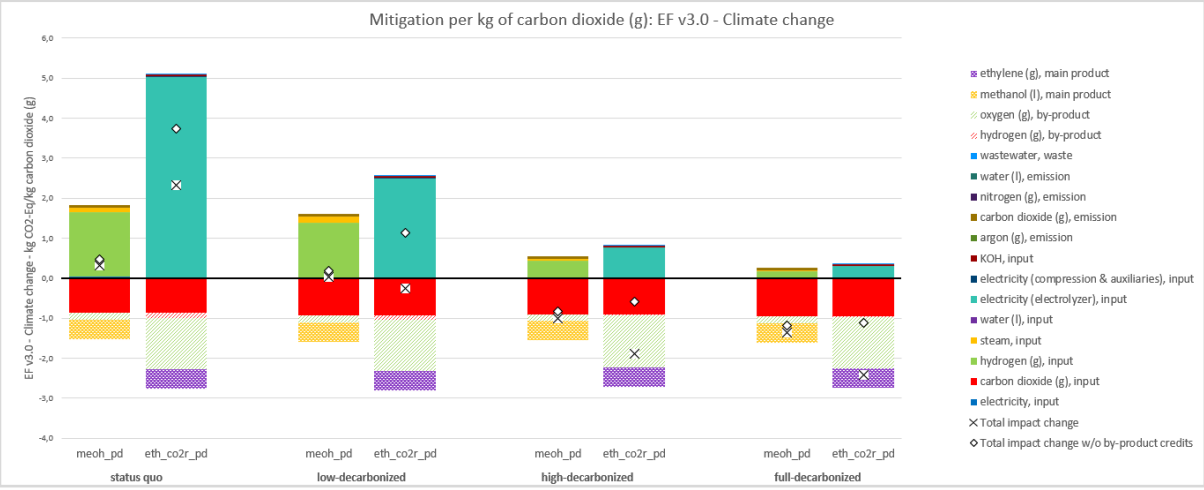


Figure 25: Exemplary Contribution Analysis result figure of a Mitigation Potential Assesment in ESTIMATe

8.3. The four decarbonization scenarios

Life Cycle Assessment (LCA) studies in the Carbon Capture and Utilization (CCU) context often exhibit diverging results due to differing supply chain assumptions. To address this, ESTIMATe employs

scenario analysis, allowing users to evaluate new processes across various supply chain contexts. This scenario approach enhances the understanding of expected environmental impacts.

ESTIMATe utilizes four scenarios representing different decarbonization levels for relevant reactants and utilities. The scenarios are based on guidelines outlined by Langhorst et al.[4] Table 1 provides an overview of the four scenarios.

Table 1: Overview of the four decarbonization scenarios in ESTIMATe, based on the scenarios from Langhorst et al.[4]. Electricity scenario source: International Energy Agency [5]

Scenario	***Status quo***	***Low-decarbonized***	***High-decarbonized***	***Full-decarbonized***
Electricity	IEA ETP reference	IEA ETP 2°C scenario, year 2030	IEA ETP 2°C scenario, year 2050	wind power
Hydrogen	steam methane reforming	alkaline electrolysis	alkaline electrolysis	alkaline electrolysis
Feedstock CO_2	coal-fired power plant	coal-fired power plant	direct air capture	direct air capture
Heat	natural gas vessel	electrode boiler	electrode boiler	electrode boiler
Steam	from heat	from heat	from heat	from heat
Natural gas	natural gas grid mix	natural gas grid mix	methanation (CO_2-based)	methanation (CO_2-based)

ESTIMATe utilizes ecoinvent data for utilities. Processes not covered by the ecoinvent database, such as methanation, are modeled based on literature sources as specified in the CCU guidelines. Steam production is modeled based on proprietary assumptions.

Interpretation: Importance of electricity for results

Electricity plays a pivotal role in CCU LCA which is reflected in the decarbonization scenarios. Not only does the electricity mix change throughout the scenarios, shifting to biomass and renewables, but there is also an increase in the overall amount of electricity required as technologies shift. In the green transition of technologies, e.g., for hydrogen production or heat generation, higher amounts of electricity become necessary. It is crucial to highlight that this change in electricity demand is not confined to a mere shift in its source but involves a substantial increase in consumption. Several impact categories are particularly sensitive to electricity variations. Understanding the reasoning can help users better understand the results in ESTIMATe, which is why we provide a few examples below.

Ionizing Radiation

Ionizing radiation impacts are dominated by nuclear electricity generation. While the share of electricity supplied by nuclear power increases only slightly in low- and high-decarbonized scenarios, the increased use of electricity for hydrogen, heat, and steam production tends to lead to high Ionizing Radiation impacts. In the full-decarbonized scenario, however, 100% wind electricity is assumed, causing ionizing radiation values to decrease.

Metal and Mineral Resource Use

The impact of electricity in categories related to metal and mineral resource use intensifies through the decarbonization scenarios, mirroring the resource-intensive surge in the

construction of renewable electricity technologies such as wind power plants. Consequently, most assessments in ESTIMATe will indicate a burden shift to metal and mineral resource use.

Land Occupation
The land occupation impact of electricity increases with increasing decarbonization. In this case, the relevant electricity production technologies are biomass technologies. While wind and solar power also affect the land occupation impacts, the influence is much smaller than that of biomass, as seen in a drop in land occupation impact from the high- to the full-decarbonized scenario.

Climate change
The shift towards renewable electricity generation technologies leads to decreasing climate change impact of electricity generation through the scenarios.

Water Use
The water use impact factor of electricity is close to static between status quo and high-decarbonized scenario since the hydropower share remains approximately the same. All variances of the water use impacts in ESTIMATe assessment results are instead related to changes in the amount of electricity consumption. When hydropower is excluded from the electricity mix in the full-decarbonized scenario, the impact in the water use category decreases substantially.

On the *scenarios* sheet in the ESTIMATe tool, you may further investigate the impacts of the decarbonization scenarios in other impact categories for all scenario products listed in Table 1.

9. Spotlight: Assessing mixtures in ESTIMATe

9.1. How to add a new mixture

The numbers in this section of the manual refer to Figure 26.

Select substances and add corresponding weight percentages [1].
Every chemical available in the *chemicals* sheet can be selected as a component of the new mixture. However, care must be taken that the sum of all weight percentages equals 1.

Click "Calculate the resulting values" [2a].
Depending on the weight percentages and molar masses of the components, the molar percentages are calculated for each component and entered to *table_mixture* [2b].
Furthermore, the mean properties of the new mixture are calculated and entered to *table_mixture_mean*. [2c]

Define a mixture name [3].
If the mixture shall be used in an assessment, the user needs to define a substance name. However, the substance name must not be the same as one of the already existing substance names in the *chemicals* sheet.

Optional: Select a connected ecoinvent process [4].
If a process exists in the *data_ei* sheet that represents the production process of the new mixture, this process can be selected to connect its characterization factors to the new mixture. This step is **optional**.

Click "Add this mixture to chemicals" [5].
After the calculation is done and the user has given the new mixture a unique substance name (i.e., a substance name that does not yet exist in *chemicals*), the new mixture can be added to the *chemicals* sheet.

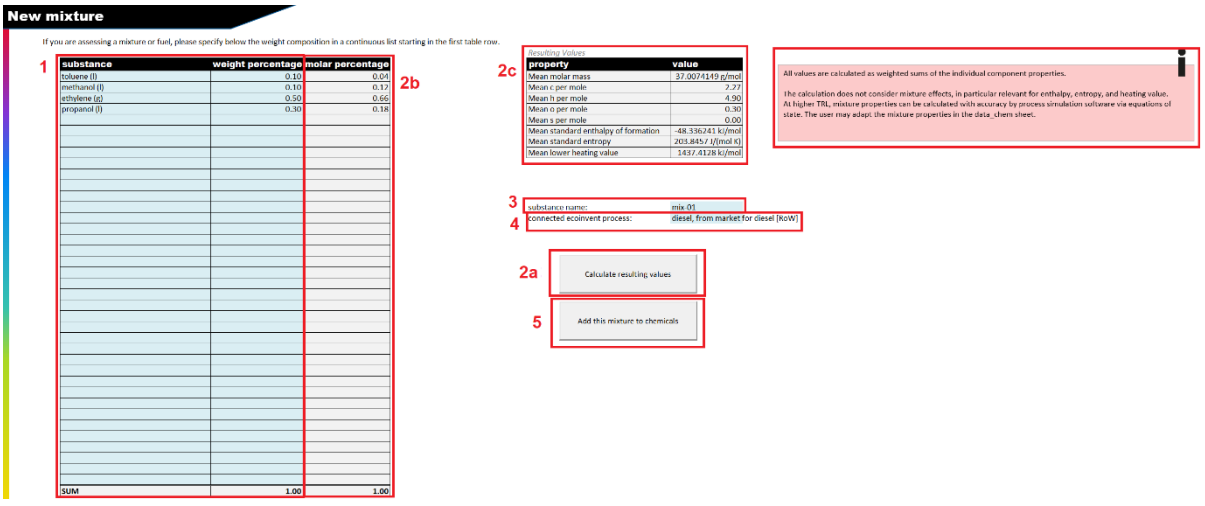


Figure 26: Overview of the New mixture sheet in ESTIMATe

9.2. Example: jet fuel in a Best-Case Assessment

In an exemplary Best-Case Assessment of a mixture, we assess the greenhouse gas reduction potential of CO_2-based jet fuel by establishing a robust lower boundary of the Global Warming Impact. For this purpose, we make ideal assumptions for the synthesis of jet-fuel via Fischer-Tropsch process and

compare the assessment results to the fossil benchmark technology, i.e., conventional kerosene production.

Introducing jet fuel as a mixture

Before creating an assessment, we first introduce "JET A-2" as a mixture in ESTIMATe as described in the Section "How to add a new mixture". For this purpose, we find the composition of jet fuel in the literature.[6] Jet fuel is a mixture of hydrocarbons of different chain lengths and configurations, many of which have numerous isomers. Thus, to model jet fuel in ESTIMATe, we use a proxy for hydrocarbons of the same chain length, distinguishing aromatics and aliphatics (cf. Figure 27).

substance	weight percentage	molar percentage
c7 aliphatics (proxy: isoheptane (2-me	0,01	
c8 aliphatics (proxy: 2-methylheptane)	0,02	
c9 aliphatics (proxy: n-nonane) (l)	0,06	
c10 aliphatics (proxy: decane) (l)	0,14	
c11 aliphatics (proxy: undecane) (l)	0,18	
c12 aliphatics (proxy: dodecane) (l)	0,15	
c13 aliphatics (proxy: tridecane) (l)	0,13	
c14 aliphatics (proxy: tetradecane) (l)	0,10	
c15 aliphatics (proxy: pentadecane) (l)	0,06	
c16 aliphatics (proxy: hexadecane) (l)	0,02	
c17 aliphatics (proxy: heptadecane) (l)	0,01	
c18 aliphatics (proxy: octadecane) (l)	0,00	
toluene (l)	0,00	
xylene (proxy: p-xylene) (l)	0,01	
trimethylbenzene (proxy: mesitylene)	0,03	
tetramethylbenzene (proxy: durene) (l	0,04	
pentamethylbenzene (l)	0,02	
hexamethylbenzene (l)	0,01	

Figure 27: JET A-2 composition as assumed in this exemplary case study. Proxy substances used for aliphatics and aromatics, respectively. Weight percentages according to [6].

We calculate the mixture properties by clicking the "Calculate resulting values" button. Finally, we name the mixture "JET A-2" and select the ecoinvent process "kerosene, from market for kerosene [RoW]" as linked ecoinvent process, before saving the mixture to the *chemicals* sheet. We can now proceed to create an assessment using the *New Assessment* sheet.

User input for Best-Case Assessment

On the *New Assessment* sheet, we specify the process name and designate the newly created mixture JET A-2 as the main product to create the new Best-Case Assessment spreadsheet. At the top of the created sheet (Figure 28), we review the assumption on intended product use to ensure that JET A-2 is assessed as a fuel on an energy content basis instead of as a chemical intermediate. Just below the intended use, the benchmark technology is already preselected from the background database.

Note that while we assess JET A-2 on an energy content basis, the unit of the ecoinvent kerosene process is kg, thus requiring a unit conversion for proper assessment. In Figure 28, ESTIMATe has adjusted the scaling factor of the benchmark process to incorporate the lower heating value of our defined substance JET A-2. Consequently, 1 MJ of JET A-2 (corresponding to 0.0228 kg of JET A-2) is compared to 0.0228 kg of kerosene. This example shows that ESTIMATe does not consider specific energy content differences between synthetic JET A-2 and conventional kerosene but assumes perfect replacement of kerosene. The user may change this assumption by adapting the benchmark scaling factor, for instance to consider a performance loss of the synthetic fuel. "1 MJ of JET A-2 is assumed to replace [0.0228*80%, i.e.,] 0.0182 kg of kerosene (from ecoinvent, see data_ei sheet)" would for instance reflect that JET A-2 reaches only 80% of the performance of conventional kerosene.

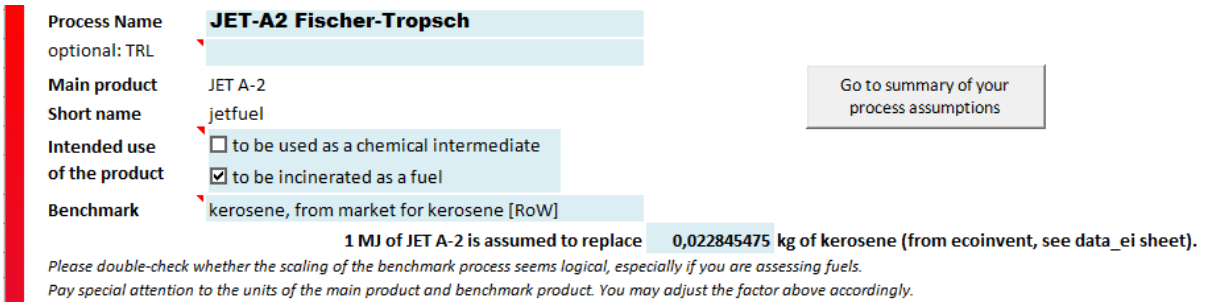


Figure 28: Header of the Best-Case Assessment sheet of JET A-2. Note that the product is intended as a fuel, and ESTIMATe has consequently adjusted the scaling factor for the benchmark process.

Next, we enter the reactants (CO_2 and hydrogen) and products (JET A-2 (pre-filled into table) and oxygen), indicating whether each component is a process input or output. We also specify the reaction type as thermochemical by checking the corresponding box. On the click of a button, ESTIMATe computes the gross reaction equation and process energy demand based on idealized assumptions, i.e., perfect CO_2 conversion, perfect selectivity, and thermodynamic minimum energy demand. Based on the gross reaction equation, ESTIMATe calculates and displays the process inventory (cf. Figure 29), i.e., the process energy and mass balance, giving us the option to double-check the data.

reference product	amount	unit	type	linked process
JET A-2	1	MJ	main product	kerosene, from market for kerosene [RoW]
carbon dioxide (g)	0,0713	kg	input	ESTIMATe feedstock carbon dioxide
hydrogen (g)	0,0034	kg	input	ESTIMATe hydrogen
oxygen (g)	0,0518	kg	emission	oxygen (g)
heat	0,5941	MJ	input	ESTIMATe heat

Figure 29: Best-Case process inventory for JET A-2 as generated by ESTIMATE.

Finally, we click “calculate LCA results”, at which point ESTIMATe generates results across four decarbonization scenarios. The results are presented both numerically and in figures which illustrate the contribution of individual process inputs and outputs to the overall environmental impact.

Results and conclusions for process development

Due to the idealized nature of Best-Case Assessments, the Global Warming Impact has only three main contributors: hydrogen production, heat generation, and the CO_2 capture process. The CO_2 capture process has a negative Global Warming Impact due to avoiding CO_2 emission to the atmosphere. Consequently, the Global Warming Impact of best-case CO_2-based JET A-2 reaches negative values in the high-, and full-decarbonized background system scenarios (Figure 30). The Global Warming Impact of the best-case JET A-2 synthesis decreases as the decarbonization level of the background system increases. Negative Global Warming Impact values are possible since ESTIMATe examines only the environmental impacts of production (“cradle-to-gate” study), and carbon captured from the atmosphere is still bound in JET A-2 at the end of the assessment scope. However, the storage of carbon in JET A-2 is not permanent, as it would be in a Carbon Capture and Storage (CCS) technology. Instead, carbon bound in JET A-2 will be emitted to the atmosphere in the product use phase, i.e., combustion. A text box adjacent to Global Warming Impact figure in ESTIMATe (Figure 31) explains temporary storage of CO_2 and specifies the amount of carbon dioxide released at the end-of-life of the product to avoid misinterpretation by the user. For instance, per MJ of JET A-2, 0.07 kg of CO_2 are emitted at the end-of-life stoichiometrically. The “cradle-to-grave” Global Warming Impact of JET A-2 production is thus always positive.

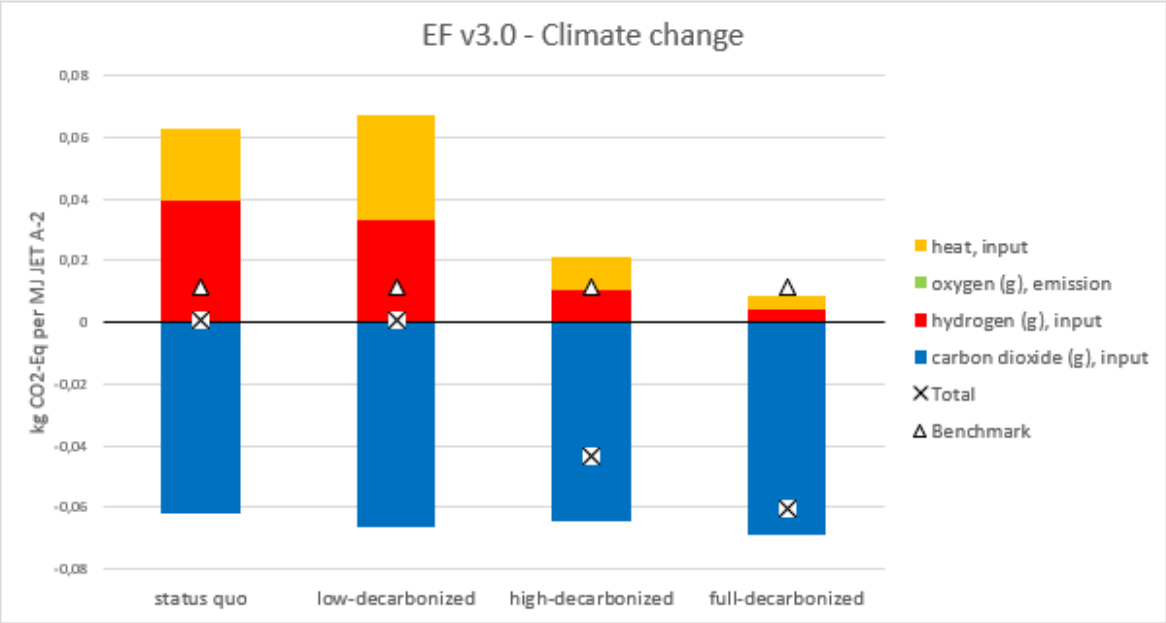


Figure 30: Global Warming Impact of the Best-Case Assessment of JET A-2 synthesis in the ESTIMATe tool. The different bars correspond to the different background system scenarios.

Carbon bound in product(s)

The product(s) may contain carbon which is captured from the environment. Upon the end-of-life of the products, all captured carbon is again released to the atmosphere. Since ESTIMATe only examines production (cradle-to-gate) environmental impacts, negative climate change impacts are possible for the assessed product(s). Please consider in your interpretation that carbon negativity is only possible if a product is permanently stored (CCS).

Assuming complete stoichiometric combustion, the main product carbon content amounts to 0,07 kg CO2 / MJ main product.

Figure 31: Bound carbon info box displayed next to JET A-2 assessment results in ESTIMATe.

Compared to the benchmark, bet-case JET A-2 synthesis achieves a lower Global Warming Impact in all scenarios, signifying that further development of the process is promising. However, environmental burden is shifted to other impact categories (Figure 32), which aligns with burden-shifting observed in renewable energy systems in general[7,8]. The main contributor to this burden-shifting is increased electricity use for hydrogen and heat production in combination with a shift towards renewable electricity sources. For instance, metal depletion impacts soar as more wind and solar power plants are introduced. Since conventional technologies have been optimized over decades and modeled in detail in LCA databases, conventional technologies often outperform new technologies in categories other than the Global Warming Impact. Still, the results in specific impact categories may be considered and, e.g., compared to criteria predefined at a company level. ESTIMATe qualitatively displays all impact categories (cf. Figure 32). For each impact category, the recommendation level from the Joint Research Center (JRC) of the European Commission is also reported as a measure for the underlying uncertainty in the impact category: the higher the recommendation level, the higher the uncertainties in a given impact category.

Summarizing, the rudimentary Best-Case Assessment of JET A-2 indicates potential to reduce climate change impact compared to conventional kerosene. A Hotspot Assessment of laboratory data for jet fuel synthesis is the logical next step to investigate whether impact reductions can be achieved in reality.

rec level	category	status quo	low-decarbonized	high-decarbonized	full-decarbonized
1	EF v3.0 - Particulate matter formation	↓	↑	↑	≈
1	EF v3.0 - Climate change	↓↓	↓↓		
2	EF v3.0 - Acidification	≈	↑	↑	≈
3	EF v3.0 - Water use	↑	↑↑	↑↑	↑
3	EF v3.0 - Material resources: metals/minerals	↑	↑↑	↑↑	↑↑
3	EF v3.0 - Energy resources: non-renewable	≈	↑	↑	↓
3	EF v3.0 - Ecotoxicity: freshwater	↓	↑	↑	≈

In reference to the to benchmark process:

↓	Impact of new process up to 10 times lower	↑	Impact of new process up to 10 times higher
↓↓	Impact of new process up to 100 times lower	↑↑	Impact of new process up to 100 times higher
≈	Impact of new process in same order of magnitude (between 80% and 150% of benchmark)	↑↑↑	Impact of new process up to 1000 times higher
	Impact of new process < 0, impact of the benchmark > 0	↑↑↑↑	Impact of new process over 1000 times higher

Figure 32: Qualitative overview of impact trends in selected impact categories in the ESTIMATe tool. Symbols indicate the performance of best-case JET A-2 synthesis compared to benchmark technology. "rec level" refers to the recommendation level from the Joint Research Center (JRC) of the European Commission, a measure for inherent uncertainty in each impact category: the higher the recommendation level, the higher the uncertainty.

10. Advanced: Adapt ESTIMATe

10.1. Update ecoinvent version

ESTIMATe uses the ecoinvent database for background LCA data. Since ecoinvent requires a license, the database is not included in the ESTIMATe upon download and needs to be imported first. See the Section "Setting up the ESTIMATe tool" for instructions on how to import ecoinvent into ESTIMATe. ESTIMATe was developed with ecoinvent Cut-off v3.8, September 2021. If you want to update the ecoinvent database to a newer version, you may download the corresponding newer file from the ecoinvent website and use the ecoinvent import functionality as described in the Section "Setting up the ESTIMATe tool". However, some changes could apply to the import of newer database versions, specifically regarding changes of naming conventions in ecoinvent.

Updates to the ecoinvent database often include changes in naming conventions for reference products. For instance, "wood chips" could be specified to "wood chips, wet, measured as dry mass" and "wood chips, dry, measured at dry mass" between ecoinvent versions. The *import_ecoinvent.xlsm* identifies relevant processes by their reference product, location, and (in some cases) process name. Changes to naming conventions thus need to be incorporated into the *Filter criteria* sheet in the *import_ecoinvent.xlsm* file, since the processes will otherwise not be included in the output sheet.

In the *Filter criteria* sheet in the *import_ecoinvent.xlsm* file:

- The "LCIA methods" table names the impact categories to include in the ecoinvent import. Make sure their names match the spelling in the .xlsx file you downloaded for your updated ecoinvent version.
- Generally, only processes with the location code "GLO" (global) and "RoW" (Rest of the World) are included in the abbreviated ecoinvent version imported into ESTIMATe. This is specified in the "locations" table.
- the "reference products (market for X)" table helps to import all "market for X" processes required in ESTIMATe, by listing all desired reference products X. Make sure all desired reference products are listed here.
- To include processes that are not called "market for X", use the second table on the *Filter criteria* sheet, in which you are able to enter a process name directly. You have the option to enter a reference product to further specify the imported process.

Once you have made sure that the filter criteria will identify all desired processes, proceed with the ecoinvent import. Once your filtered ecoinvent sheet is created, copy and paste it into your ESTIMATe file. Make sure there is only one sheet called "*data_ei*" and that the *data_ei* sheet includes your updated data. Do not forget to update your ESTIMATe scenario sheet as described in the Section "Setting up the ESTIMATe tool". ESTIMATe should now work as usual and use your updated database. If it does not, it could help to double-check the following points:

- The table on the *data_ei* sheet is called "table_data_ei" (check by selecting any cell within the table and then navigating to the "table" context menu at the top of the page)
- On the *Processes* sheet in ESTIMATe, the G column should automatically have updated to a list of processes of your new ecoinvent version. If that did not happen, you may update the list in the G column manually.

If you update to a new ecoinvent version, make sure you also update the *scenarios* sheet to keep your background data consistent. When calculating the impacts for the *scenarios* sheet, you might get an error message if there were changes in process naming in ecoinvent. The import_ecoinvent sheet will

alert you which processes required for the scenario calculation cannot be found in the ecoinvent database, so you can adapt the names to reflect the newest naming convention.

Please consider emptying your ESTIMATe version of all assessments in the *data_own* database since after the update, their results will be outdated. Recalculate any existing assessment to update the results to the novel background database.

10.2. Add a substance to ESTIMATe

To add a new substance that is not a mixture, go to the "chemicals" sheet in ESTIMATe.

Enter the name of the new substance on the bottom left, right below the table (cf. Figure 33). The naming convention is: [trivial name] ([state of matter]), where the state of matter is either g – gaseous, l – liquid, or s – solid.

Excel automatically extends the table by a row to include the new substance.

	substance	molecular formula	trivial name	phase	molar mass	c per	h per	o per	n per	melting point
104	water (g)	$H_2O_{(s)}$	water	g	18,02 g/mol	0	2	1	0	
105	water (l)	$H_2O_{(l)}$	water	l	18,02 g/mol	0	2	1	0	
106	xylene (proxy: p-xylene) (l)	$C_8H_{10(l)}$	xylene (proxy: p-xylene)	l	106,2 g/mol	8	10	0	0	
107	nitrogen (g)									

Figure 33: Example for adding a new row in the chemicals sheet

Fill in the remaining data as well as you can. At a minimum, fill in the molar mass and molecular composition.

- For chemical properties, refer to, e.g., the NIST database[9].
- ESTIMATe assumes standard conditions (25°C, 1 bar)
- For a linked ecoinvent process, select a process name from the first column on the "data_ei" sheet. This process will be the default assumed process for the new substance.
- To consider the impacts of emitting the new substance in LCA studies, characterization factors are necessary. You can find these characterization factors in the "LCIA implementation" table provided by ecoinvent[a] (cf. Figure 34). If you find characterization factors for your substance, set the "characterization factors exist?" column on the "chemicals" sheet to True and enter the characterization factors into their corresponding impact column on the "chemicals" sheet.

	A	B	C	D	E	F	G
1	Method	Category	Indicator	Name	Compartment	Subcompartment	CF
2296	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	air	unspecified	0,42
2297	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	soil	agricultural	0,42
2298	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	soil	forestry	0,42
2299	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	soil	industrial	0,42
2300	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	soil	unspecified	0,42
2301	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	water	ground-	0,42
2302	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	water	ocean	0,42
2303	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	water	surface water	0,42
2304	CML v4.8 2016 no LT	eutrophication no LT	eutrophication (fate not incl.) no LT	Nitrogen	water	unspecified	0,42
6139	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	air	unspecified	0,42
6140	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	soil	agricultural	0,42
6141	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	soil	forestry	0,42
6142	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	soil	industrial	0,42
6143	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	soil	unspecified	0,42
6144	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	water	ground-	0,42
6145	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	water	ground-, long-term	0,42
6146	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	water	ocean	0,42
6147	CML v4.8 2016	eutrophication	eutrophication (fate not incl.)	Nitrogen	water	surface water	0,42

Figure 34: Screenshot of the LCIA implementation table provided by ecoinvent

[a] Download the impact category information in xlsx Format from the ecoinvent website:

1. Log in to the ecoinvent website using your credentials.
2. Navigate to the "Files" tab.
3. Under "supporting documents" click on the file with the ending "LCIA_implementation.7z" to start the download.
4. Unpack the zip folder and find the unpacked "LCIA Implementation X.Y.Z.xlsx"

10.3. Add impact categories

Users may add impact assessment methods to the ESTIMATe tool. This procedure involves modifications across multiple sheets in the Excel file and may take some time to complete. Additionally, please exercise caution as there is a possibility of unintentional changes that could impact existing data. Take your time, double-check your actions, and consider creating a backup before proceeding with this process.

Select which method will be added

1. Download the impact category information in xlsx Format from the ecoinvent website
    1. Log in to the ecoinvent website using your credentials.
    2. Navigate to the "Files" tab.
    3. Under "supporting documents" click on the file with the ending "LCIA_implementation.7z" to start the download.
    4. Unpack the zip folder.
2. Find the desired impact assessment method in Column A of the unpacked "LCIA Implementation X.Y.Z.xlsx"

	A	B	C	D
1	Method	Category	Indicator	Indicator Unit
331	IPCC 2013 no LT	climate change no LT	global temperature change potential (GTP20) no LT	kg CO2-Eq
333	IPCC 2013 no LT	climate change no LT	global warming potential (GWP20) no LT	kg CO2-Eq
335	IPCC 2013	climate change	global temperature change potential (GTP20)	kg CO2-Eq
337	IPCC 2013	climate change	global warming potential (GWP20)	kg CO2-Eq
341	IPCC 2021 no LT	climate change no LT	global warming potential (GWP20) no LT	kg CO2-Eq
346	IPCC 2021 no LT	climate change: biogenic no LT	global warming potential (GWP20) no LT	kg CO2-Eq
350	IPCC 2021 no LT	climate change: biogenic, including SLCFs no LT	global warming potential (GWP20) no LT	kg CO2-Eq
354	IPCC 2021 no LT	climate change: fossil no LT	global warming potential (GWP20) no LT	kg CO2-Eq
358	IPCC 2021 no LT	climate change: fossil, including SLCFs no LT	global warming potential (GWP20) no LT	kg CO2-Eq
361	IPCC 2021 no LT	climate change: including SLCFs no LT	global warming potential (GWP20) no LT	kg CO2-Eq
365	IPCC 2021 no LT	climate change: land use no LT	global warming potential (GWP20) no LT	kg CO2-Eq
369	IPCC 2021 no LT	climate change: land use, including SLCFs no LT	global warming potential (GWP20) no LT	kg CO2-Eq
373	IPCC 2021	climate change	global warming potential (GWP20)	kg CO2-Eq
378	IPCC 2021	climate change: biogenic	global warming potential (GWP20)	kg CO2-Eq
382	IPCC 2021	climate change: biogenic, including SLCFs	global warming potential (GWP20)	kg CO2-Eq
386	IPCC 2021	climate change: fossil	global warming potential (GWP20)	kg CO2-Eq

Add the new method to the ecoinvent import

1. In the "import_ecoinvent.xlsx" file, on the *Filter criteria* and *Filter criteria elec* sheets, add your desired impact assessment method to the LCIA methods table. Use the name from the above-mentioned LCIA_implementation provided by ecoinvent.
2. Follow the instructions in Chapter 2 of this manual to create new versions of the *data_ei* and *scenarios* sheets and add them to ESTIMATe
    a. Make sure the created sheets contain your desired impact categories.
    b. When copying the new data to the *scenarios* sheet in ESTIMATe, please avoid overwriting the final column in the scenario tables, as it is utilized for figure creation in ESTIMATe. To prevent overwriting, insert an empty column in the middle of the scenario tables for each category that needs to be added.

Add each category of the new method to the *impact categories* sheet

The *impact categories* sheet contains information on each impact category. It is important that each impact category is listed in the table for calculations to work correctly. For each impact category,

- the "name" is a short name for the impact category, but must not necessarily be unique
- the "combined name" is the unique name used in ESTIMATe tables such as data_ei or the scenarios tables. It includes all pieces of information available for the impact category.
- The columns "Unit", "impact assessment method", and "impact category" include individual pieces of information used for instance for figure creation.
- If available, you may add a level of recommendation.
- The columns "in simplified EF overview" and "in user selection" form the basis of category grouping for the overview figures on Best-Case and Hotspot Assessment sheets.

Add characterization factors for each category to data_chem

1. On the *chemicals* sheet, add the new impact categories as columns. Make sure the columns have the same order and names as on the data_ei and scenarios sheets.
2. In the LCIA_implementation Excel file provided by ecoinvent and mentioned above, look up the characterization factors for the substances in *chemicals* in each added category. Add the characterization factors on the *chemicals* sheet.
3. For carbon-containing substances without climate change characterization factors, calculate stoichiometric combustion CO_2 emissions per kg of the substance as climate change characterization factor.

Add columns/rows to all tables displaying LCA results

Add the new impact categories as columns in the following tables. Make sure the columns have the same order and names as on the data_ei and scenarios sheets:

- All four results tables on the Best-Case Assessment Template and any existing Best-Case Assessments
- All four results tables on the Hotspot Assessment Template and any existing Hotspot Assessments
- All eight contribution analysis tables at the bottom of the Mitigation Potential Assessment Template and any existing Mitigation Potential Assessment (starting from line 250)
- The data_own table on the *data_own* sheet

Add the new impact categories as rows in the following tables:

- The impact category overview table on the Best-Case Assessment Template and any existing Best-Case Assessments
- The table_results_all_cats starting from line 349 on the Best-Case Assessment Template and any existing Best-Case Assessments
- The impact category overview table on the Hotspot Assessment Template and any existing Hotspot Assessments
- The table_results_all cats starting from line 364 on the Hotspot Assessment Template and any existing Hotspot Assessments
- The two results overview tables on the Mitigation Potential Assessment Template and any existing Mitigation Potential Assessment

Check whether dropdown menus of impact categories were extended automatically

There is a category dropdown menu at the top of the *scenarios* sheet where you can check whether it includes the new categories. If it does not contain the new categories, right click the cell with the dropdown menu and extend the reference range for the dropdown manually. Do the same for all other dropdown menus with impact categories, located with the contribution analysis results on all Assessment templates.

If your added impact categories come first or last in the order of impact categories

In a few places in ESTIMATe, the code determines the first and last column of impact data in tables by finding impact categories by their name. In particular, ESTIMATe expects the first column with impact data in tables such as data_own and data_ei to be called "EF v3.0_acidification_accumulated exceedance (ae)_[mol H+-Eq]" and the last column to be called "ReCiPe Midpoint (H) V1.13_water depletion_WDP_[m3 water-.]". If your added impact categories come first or last in the order of columns, it is an easy fix:

1. In the ESTIMATe VBA project, search for “acidification”/“water depletion”, respectively, and replace the former first/last column’s impact category name with the current first/last column’s name. Use the “combined name” format of the impact category name, as used in, e.g., data_ei.
2. On the *scenarios* sheet, in the last column of the scenarios tables (used for figure creation), adjust the formulas located in the cells to include the correct first and last column names.

11. Troubleshooting Tips

1. **Do not change the sheet names (or any other variable names)**
   The code behind ESTIMATe refers to objects on the sheet by referring to their names. This includes tables located on all sheets in ESTIMATe. In particular for assessment sheets, there are naming conventions applied when creating a new assessment. These naming conventions use the short name you have given to the sheet and are used throughout the ESTIMATe tool. For this purpose, NEVER CHANGE A SHEET NAME in ESTIMATe, and never change the names of variables, tables, or other objects.

2. **Do not delete the assessment templates or other hidden sheets**
   While you never work directly on the assessment template sheets, they are required for ESTIMATe to work correctly. The same holds for the *Processes* and *DropDown* sheets.

3. **Macros must be enabled for ESTIMATe to work**
   To enable macros, click the "enable macros" button in the yellow ribbon when opening the ESTIMATe Excel file. If you do not see the yellow ribbon, close the ESTIMATe Excel file again, then right-click it, go to "Properties" and check "Unblock" under "Security". Reopen ESTIMATe.

4. **In case you need to deactivate worksheet protection**
   You can deactivate worksheet protection using the password "abcde". Please do not change the password when protecting the sheet again since macros use the password too. Also, please note that worksheets are protected on their activation, so if you switch sheets, protection is active again.

5. **Buttons/Checkboxes unclickable**
   Apart from disabled buttons/checkboxes, indicated by grey font, all buttons and checkboxes should be clickable at all times. However, the Excel Forms Controls used to implement buttons and checkboxes can be unreliable at times. Try to close and reopen ESTIMATe. If that does not fix the issue, try moving the affected button/checkbox slightly. To move an object, you must be in Excel design mode, available from the Excel Developer ribbon.

6. **Errors occurring in the VBA code**
   If you want to inspect the VBA code, go to the Excel Developer Ribbon and click "Visual Basic". Refer to the Technical Manual (cf. in this document: Part 2: Technical Manual) for explanations of functions and their location.
   a. If you are looking for mistakes in the VBA code, disable Error handlers ("On Error GoTo") in the code since they will not let you pinpoint the exact location of the error. However, they are useful to not let the tool crash when errors occur.
   b. If you work with the VBA code, run into an error, and afterwards cannot work with the tool correctly anymore, try the following:
      i. In the direct Window, run:
         1. Application.ScreenUpdating = True
         2. Application.EnableEvents=True
      ii. Switch sheets, and then switch back (to re-define all variables on the sheet)

Part 2: Technical Manual

I. Introduction to VBA code

This Section enumerates all VBA (Visual Basic for Applications) functions used in ESTIMATe. To access the code, click on “Visual Basic” in the “Developer Tools” tab in Excel. You might first have to enable the “Developer Tools” tab in the Excel options.

In ESTIMATe, some functions are defined workbook-wide, and some are only available on individual Worksheets. For each function documented below, the location is specified first. In the Visual Basic explorer window, you can access the code on individual Worksheets under “Microsoft Excel Objects”, and general code under “Modules” (cf. Figure 35).

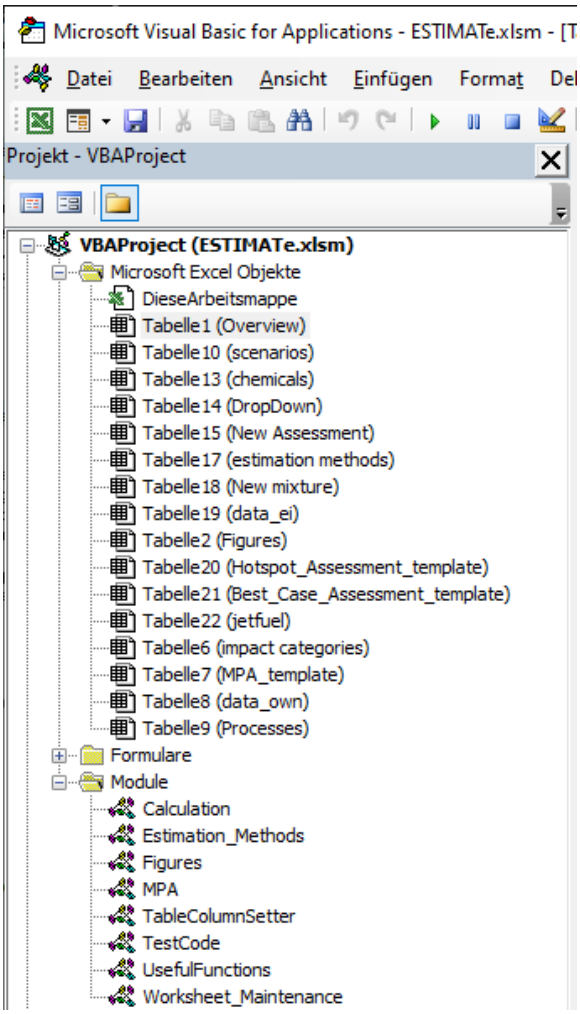


Figure 35: Structure of ESTIMATe code in Visual Basic for Applications editor

II. New Assessment

Worksheet_Activate on *New Assessment*

Location: Worksheet – New Assessment

- The *New Assessment* sheet is protected.

Create_New_Assessment_Click (Button)

Location: sheet – New Assessment

This function reads user inputs from the new assessment sheet and creates a new sheet from the templates (Best Case, Hotspot, or Mitigation Potential) according to user specifications. If the sheet to be created already exists, an error message appears, and the code is terminated.

First, the template is copied. Then, importantly, the defined Excel tables on the templates are renamed to incorporate the short name of the new assessment. This renaming process is crucial for ESTIMATe functions to work properly. The user specifications from the *New Assessment* sheet are entered into the new sheet. For Best Case and Hotspot Assessment studies, a benchmark process in the *chemicals* sheet is searched and, if found, entered into the new sheet.

Calls *benchmark_assumption.*

Worksheet_Change on *New Assessment* sheet

Location: Worksheet – New Assessment

- Toggles the New Assessment Button to be enabled (=clickable) only if all relevant fields are filled in.
- If Mitigation Potential Assessment is chosen as the study goal, disables the “Choose main product” cell, since the input is not required for Mitigation Potential Assessment studies.

III. New mixture

Worksheet_Activate on *New mixture* sheet

Location: MS Excel Objects – New mixture

Once the *New mixture* sheet is activated, *table_mixture*, *table_mixture_mean* and *table_chemicals* are defined as variables, along with their corresponding columns. The *New mixture* sheet is then protected.

Worksheet_Change on *New mixture* sheet

Location: MS Excel Objects

If a component or its weight percentage is changed in, deleted from, or added to *table_mixture*, clear the formerly calculated molar percentages in *table_mixture* and the calculated mean properties from *table_mixture_mean*.

calculate_mixture

Location: module - Calculation

called from: MS Excel Objects – New mixture

This function calculates the mean properties of a mixture based on components and their weight percentages listed in *table_mixture*. Property data of components is taken from *table_chemicals.*

First, the mean properties of previous calculations are cleared from *table_mixture_mean*.

Check prerequisites:

- If the sum of the weight percentages does not equal 1, the user is notified, and the procedure is interrupted.
- If the component entries are not continuous, i.e., there are empty rows in *table_mixture*, the user is informed, and the procedure is interrupted.

Calculation steps:

- calculate the mean molar mass of the mixture:
  - mean molar mass = 1 / *sum* (weight percentage i * molar mass i)
- calculate the molar percentages of the components:
  - molar percentage i = (mean molar mass / molar mass i) * weight percentage i
- calculate all mixture mean properties: mean c/h/o/s per mole, mean standard enthalpy of formation, mean standard entropy, mean lower heating value.
  - mean property = *sum* (molar percentage i * property i)

add_mixture

Location: module – Calculation

This function adds the mean properties of a calculated mixture (see *calculate_mixture*) to *table_chemicals*. In addition to the mixture's properties, a substance name (that is unique to all other substance names in *table_chemicals*) is required. Optionally, an ecoinvent process can be linked to the mixture (and, thus, to its entry in *table_chemicals*).

Check prerequisites:

- If a substance name for the mixture has not been set, the user is notified, and the procedure is interrupted.
- If the set substance name for the mixture already exists in *table_chemicals*, the user is notified, and the procedure is interrupted.

Adding all mean properties of the mixture to *table_chemicals*:

- Substance and molecular formula are both filled by the set mixture name.
- Mean molar mass, mean c/h/o/s per mole, mean standard enthalpy of formation, mean standard entropy, mean lower heating value.
- If the user has set a connected ecoinvent process for the mixture, it is added to *table_chemicals.*
- "Is mixture?" is set to *True* to indicate in *table_chemicals* that this substance is a mixture that has been set in the *New mixture* sheet.

Button_mixture_resulting_values_Click()

Location: MS Excel Objects: New Mixture

calls *calculate_mixture* which calculates the mean properties of a mixture based on components listed in table_chemicals and their added weight percentages.

Button_mixture_add_to_chemicals_Click()

Location: MS Excel Objects: New Mixture

calls *add_mixture* which adds a defined mixture to the chemicals sheet from the new mixture sheet.

IV. Best Case and Hotspot Assessment

Worksheet_Activate *on Best-Case Assessment sheets*

Location: Worksheet – Best_Case_Assessment_template (and any instances of Best-Case Assessments)

- Calls *setColumns* to give useful short variable names to all tables and columns on the sheet.
- hides and disables checkboxes that are not relevant to Best-Case assessments but would cause calculation codes to throw errors if they did not exist. Namely:
    - Checkbox_skip_stoic (only stoichiometric heuristics considered in BCAs)
    - CheckBox_Hischier_Gendorf (no estimation methods supported in BCAs)
    - CheckBox_PI_manual (only process inventory based on stoichiometry is allowed)
    - CheckBox_allocation (allocation multifunctionality approach not supported in BCA)
- finally, active BCA sheet is protected.

Worksheet_Activate on *Hotspot Assessment sheets*

Location: Worksheet – Hotspot_Assessment_template (and any instances of Hotspot Assessments)

- Calls *setColumns* to give useful short variable names to all tables and columns on the sheet.
- active HSA sheet is protected.

Worksheet_Change on *Best-Case Assessment sheets*

Location: Worksheet – Best_Case_Assessment_template (and any instances of Best-Case Assessments)

- Updates the process assumptions box at the top of the assessment sheet by calling *UpdateProcessAssumptions.*
- If changes are made to the benchmark process or scaling factor, calls *benchmark_assumption.*
- If changes are made in any input cell, clears all results that depend on the changed input.
- If an impact category is chosen from the dropdown menu next to the contribution analysis, calls *make_figure_current_ca.*

    - If the impact category name contains “Climate change”, toggles TextFrame with information on bound CO_2.
- If changes are made to the process inventory (changes can only be made to the *type* or *linked process* column), auto-fills linked processes where possible and creates dropdown menus.
    - If a reference product is deleted from the process inventory, deletes any dropdown menu and entry in the “linked process” of that reference product.
    - If a reference product type is set to “input” or “by-product”,
        - generates a dropdown menu including all processes in *data_ei*, *scenarios*, and *data_own*
        - looks for a predefined linked process in *chemicals* by searching for the exact reference product name. Also enters predefined processes for the reference products “heat”, “steam”, “electricity”, and “cooling water”.
    - If a reference product type is set to “emission”,
        - Deletes any dropdown menu from the “linked process” cell.
        - If the reference product exists in *chemicals* AND characterization factors exist for that reference product (identified by the corresponding column in *chemicals*), writes the reference product name into the “linked process” cell to indicate that emission data on the substance was found. Otherwise, writes “[not characterized]” to “linked process” cell.
    - If a reference product type is set to “waste”, generates a dropdown menu including only waste treatment processes from *data_ei.*

Worksheet_Change on *Hotspot Assessment sheets*

Location: Worksheet – Hotspot_Assessment_template (and any instances of Hotspot Assessments)

- Updates the process assumptions box at the top of the assessment sheet.
- If changes are made to the benchmark process or scaling factor, calls *benchmark_assumption.*
- If changes are made in any input cell, clears all results that depend on the changed input.
- If changes are made to the allocation factors in *tbl_allocation*, checks whether the allocation factors add up to 100% and colors in cells accordingly.
- If an impact category is chosen from the dropdown menu next to the contribution analysis, calls *make_figure_current_ca.*
    - If the impact category name contains “Climate change”, toggles TextFrame with information on bound CO_2.
- If a by-product is declared in the process inventory, unhides *CheckBox_allocation* and fills names of the main product and all by-products into *tbl_allocation.*
    - Allocation calculations support up to four by-products. If more by-products are defined, notifies user and terminates code.
    - If all by-products are deleted, hides *CheckBox_allocation* and clears *tbl_allocation.*
- If changes are made to the process inventory, auto-fills linked processes where possible and creates dropdown menus.
    - If a reference product is deleted from the process inventory, deletes any dropdown menu and entry in the “linked process” of that reference product.
    - If a reference product type is set to “input” or “by-product”,
        - generates a dropdown menu including all processes in *data_ei*, *scenarios*, and *data_own*

        - looks for a predefined linked process in *chemicals* by searching for the exact reference product name. Also enters predefined processes for the reference products “heat”, “steam”, “electricity”, and “cooling water”.
    - If a reference product type is set to “emission”,
        - Deletes any dropdown menu from the “linked process” cell.
        - If the reference product exists in *chemicals* AND characterization factors exist for that reference product (identified by the corresponding column in *chemicals*), writes the reference product name into the “linked process” cell to indicate that emission data on the substance was found. Otherwise, writes “[not characterized]” to “linked process” cell.
    - If a reference product type is set to “waste”, generates a dropdown menu including only waste treatment processes from *data_ei.*

calculate_stoichiometry

Location: module – calculation

This Function calculates the stoichiometric reaction equation from the reactants (divided into inputs and outputs). The calculation of stoichiometric coefficients uses a linear system of equations of the form $A \cdot x = y$, where x contains the stoichiometric coefficients.

The function scales the equation to the main product and takes the user-specified carbon conversion into account.

Step 1: Prerequisite check in tbl_stoic

- check if every substance has a type (input/output). If not: alert user and terminate code.

Step 2: Calculation

- Read the elementary composition of reactants into a matrix (rows=substances, columns=elements), with input rows receiving negative sign
- Delete empty columns (=elements not taking part in the reaction)
- Add a scaling column (1 0 0 … 0) for scaling of the reaction equation to the main product (if the output substances contain one [or more] carbon-containing substances, the main product needs to be carbon-containing)
- *If required*: declare selectivities.
    - Determine whether any outputs (other than the main product) contain carbon.
        - if the main product is not carbon-containing but at least one carbon-containing product exists, the user is asked to create a new assessment with a carbon-containing main product.
    - If any outputs (other than the main product contain carbon, a message box asks the user for a carbon selectivity towards each carbon-containing output, including the main product. Then, both the selectivity and the number of C atoms of each corresponding carbon-containing by-product are added as columns to the right-hand side of the matrix.
    - Limitation for the selectivity calculation: there may be only one carbon-containing input substance.
- *If required*: eliminate linear dependencies.

    - If the number of elements = number of reactants, check for linear dependencies between stoichiometric coefficients in reduced matrix matRed
    - A Gauss elimination algorithm[b] is applied using column pivoting to prevent division by 0. After running the algorithm, linear dependent columns are located at the end of the reduced matrix (matRed) and then eliminated.
- Transpose the resulting square matrix (matRed) to receive matrix A
- Invert matrix A
- Solve the equation $A^{-1} \cdot y = x$ with $y = (1,0,0, \dots 0)$ (1 is for scaling) to obtain the stoichiometric coefficients in vector x
- If carbon conversion is specified, apply carbon conversion (=yield) to the stoichiometric coefficients.
- Calculate the reaction enthalpy (for thermochemical reactions) or Gibb's free reaction enthalpy (for electrochemical reactions) using the stoichiometric coefficients and chemical properties.
    - Assumption: standard pressure and temperature for all properties; no mixture effects considered

calculate_process_inventory

Location: module – calculation

This function provides an inventory of all reference products that are needed for the stoichiometric reaction equation calculated in the previous step. The amount, unit, and type (either input or emission) of each reactant and utility are set. If available, the calculation offers a predefined linked process for each input which can also be manually changed.

Reference products with the type 'emission' are linked to their corresponding row in the *chemicals* sheet that provides characterization factors for the emission of substances if available. If a corresponding row in the *chemicals* sheet does not provide characterization factors for an emission, the environmental impacts are set to zero during the contribution analysis in the "*calculate_contribution_analysis*" function. If a reference product in the process inventory does not exist in table_chemicals, but is declared as an emission, its linked process is set to "not characterized" and the environmental impacts are set to Zero in the *"calculate_contribution_analysis"* function.

Linked processes for waste products always need to be set manually.

The function scales the amount of each reference product necessary to 1 kg or 1 MJ of the predefined main product (depending on if the main product is intended to be incinerated as fuel (-> functional unit: 1 MJ) or to be used as a chemical intermediate (-> functional unit: 1 kg)).

Thermochemical/electrochemical reactions: If the actual reaction enthalpy/Gibb's energy demand is above 0 kJ/mol main product, it is converted to a heat/electricity demand (in MJ or kWh **per functional unit**) and added to the process inventory.

If "Gendorf assumptions" are selected by the user:

[b] https://en.wikipedia.org/wiki/Gaussian_elimination

- 0.2 wt.-% of every input material is assumed to be emitted to air (-> gaseous). The rest of all unreacted inputs (= all unreacted inputs - gaseous Complement) is assumed to be emitted to water (-> liquid).
    - prerequisite: substance is available in both gaseous and liquid state of matter in table_chemicals.
- per **1 kg main product**, the following inputs are assumed:
  0.416 kWh electricity
  2.15 MJ heat
  0.2 MJ steam
  24 kg water
    - If the main product is to be incinerated as fuel (-> functional unit: 1 MJ), the amounts of electricity, heat, steam and water input need to be adjusted using the main product's molar mass and lower heating value!

calculate_contribution_analysis

Location: module – calculation

Step 1: Preparation - Process Inventory Check – terminate calculation if errors detected.

- Does every reference product in the process inventory have a type?
- Are valid amounts specified for each entry?
    - if not: Ask if the user would like to proceed anyway. The invalid amount(s) would be set to Zero and, thus, their environmental impacts would be set to Zero as well (in step 3).
- Are characterization factors available for each emission?
    - if not: A note with a red background appears to the right of the process inventory table indicating that "some substances are not characterized". Furthermore, the environmental impacts of these not characterized emissions are set to Zero in the calculation (in step 3).
- Do all linked processes actually exist?
- Are any linked process cells empty?
- Does the specified unit match the unit of the linked process (ESTIMATe/data_own/ ecoinvent)?
    - if not: Ask if the user would like to proceed anyway. The environmental impacts of the regarding reference products would be set to Zero (in step 3).
- Are input and output mass equal? (only reference products with the unit *kg* are considered for the mass balance)

Step 2: Allocation

- if by-product(s) exist and the user chooses to solve the multifunctionality using allocation (indicated by allocation checkbox =True), the user needs to specify:
    - an *allocation criterion* (e.g., economic value of each reference product)
    - *allocation factors* for each of the (main and by-) products (allocation factors need to sum up to 100%)
- No actual calculation regarding the contribution analysis takes place in this section. The code **only checks**, if:
    - allocation factors are specified for each entry (main product and by-products),

- all specified allocation factors sum up to 100%,
- the user specified an allocation criterion.

Step 3: Calculation

- all reference products, amounts, units, types, and linked processes are transferred to each of the four contribution analysis tables (status quo [sq], low-decarbonized [ld], high-decarbonized [hd], full-decarbonized [fd])
- if a unit or amount in the process inventory is invalid (yellow background), but the user chooses to proceed the calculation, the environmental impacts of this particular reference product are set to Zero.
- the calculation of the environmental impacts is conducted for the same row of ALL contribution analysis tables (sq, ld, hd, fd) and for all impact categories simultaneously and primarily depends on the *type* of the current reference product:
  - input: **env. impact = process impact * amount**
    - If the linked process is an *ESTIMATe* process (i.e., linked process string starts with "ESTIMATe "), its process impacts are taken from the *scenarios* sheet.
    - If the linked process is an OWN process (i.e., linked process string starts with "OWN "), its process impacts are taken from the *data_own* sheet.
    - If the linked process is an ecoinvent process, its process impacts are taken from the *data_ei* sheet.
  - by-product: **env. impact = process impact * amount * (-1)**
    - Reasoning for (-1): By-products receive a credit ("avoided burden") for avoiding conventional production
    - If the linked process is an *ESTIMATe* process (i.e., linked process string starts with "ESTIMATe "), its process impacts are taken from the *scenarios* sheet.
    - If the linked process is an OWN process (i.e., linked process string starts with "OWN "), its process impacts are taken from the *data_own* sheet.
    - If the linked process is an ecoinvent process, its process impacts are taken from the *data_ei* sheet.
  - waste: **env. impact = process impact * amount**
    - all waste treatment processes are *ecoinvent* processes. Thus, its process impacts are taken from the *data_ei* sheet.
  - emission: **env. impact = characterization factor * amount**
    - If the entry in the linked process cell says *"[not characterized]"*, the environmental impacts of the regarding reference product are set to **Zero**.
    - If the substance name of the reference product exists in the "substance" column of *table_chemicals* and if the corresponding cell in the "characterization factors exist?" column of *table_chemicals* is "TRUE", the characterization factors are taken from the *chemicals* sheet for the substance's linked process.
- If allocation is used as a multifunctionality approach, "cache" 100% of process impacts (not yet allocated impacts) below the TotalsRowRange. After that, the corresponding shares of the total impacts are allocated to the main and all by-products by adding rows to the contribution analysis tables. Further, an indication of the share of impact allocated to each product is added to the left of the contribution analysis tables.
- Bound CO_2 in main product and by-products is calculated and stored on the Worksheet (in *varBoundCO2main* and *varBoundCO2byp* that are both lying behind the *current_ca figure* of the current contribution analysis).

- For each category and in each contribution analysis table calculate the sum including avoided burden(s)/allocation and enter into the TotalsRowRange, resulting in the total impacts of the studied main product.
- The sum of the environmental impacts for each impact category (i.e., the total impacts of the studied main product) is transferred to the overall results table of the contribution analysis (*tbl_results_all_cats*).

benchmark_assumption

Location: module – Worksheet_Maintenance

This function calculates the benchmark scaling factor, i.e., the amount of the benchmark product that is assumed to be replaced by the selected main product. In addition, the benchmark impacts are calculated using the *add_and_divide_benchmark* function.

benchmark_assumption is called when the benchmark process is changed, or when the functional unit of the assessment changes (by clicking the checkboxes fuel/intermediate)

First, check prerequisites:

- If no benchmark process is selected, the benchmark impact columns in *table_results_all_cats* are cleared, and the user is asked to add a valid benchmark process.
- If the selected benchmark process is not valid (i.e., the selected benchmark process does not exist in either database (comparison using the *DropDown* sheet)), the user is asked to adjust the selection.

If possible, calculate a default scaling factor:

- When considering the main product's use as a chemical intermediate, we assume that 1 kilogram of the main product can replace a specific quantity of the chosen benchmark. Conversely, if the user intends to incinerate the main product as a fuel, we assume that 1 megajoule (MJ) of the main product can replace a specific quantity of the chosen benchmark.
- This "specific quantity of the chosen benchmark", i.e., scaling factor, can be manually adjusted by the user. However, if feasible, the function provides a default scaling factor for the selected benchmark. This automatic calculation considers the functional unit, the unit of the benchmark process, as well as the molar mass and lower heating value of the main product.

Using the *scale_benchmark_impacts* function, the benchmark impacts are calculated.

scale_benchmark_impacts

Location: module – Calculation

This function calculates the benchmark impacts and writes them to *table_results_all_cats*. If no benchmark process is defined, the benchmark impact columns in *table_results_all_cats* are cleared.

Check prerequisites:

- If the user sets a benchmark scaling factor while no benchmark process is yet selected, both the scaling factor and all benchmark impacts in the *table_results_all_cats* are cleared. After that, the user is asked to select a benchmark process first.

- If the user deletes a previously set benchmark process, both the scaling factor and all benchmark impacts in the *table_results_all_cats* are cleared. After that, the user is asked to select a new benchmark process.
- If the selected benchmark process is not valid (i.e., the selected benchmark process does not exist in any database as determined by the list on the *DropDown* sheet), the user is asked to adjust the benchmark process. In addition, all benchmark impacts in the *table_results_all_cats* are cleared.

To calculate the benchmark impacts, first, the impact values of the corresponding benchmark process are extracted from the *scenarios*, *data_own,* or *data_ei* sheet. After that, each value is divided by the benchmark scaling factor. However, if the benchmark scaling factor is not a numeric, positive value, all benchmark impacts in *table_results_all_cats* are cleared, and the user is asked to select a proper scaling factor.

add_to_data_own

Location: module – Calculation

Writes study assumptions and results from a hotspot assessment to the *data_own* sheet, thereby adding the study results as a process to the background database.

Check prerequisites:

- If no results have been calculated in the hotspot assessment, the user is asked to finish the assessment and the code is terminated.
- If a process of the same name already exists in *data_own*, the user is asked whether to override the existing process. If "no" is selected, the code is terminated.

The following information is written to the database:

Main product, process name, sheet name, assessment goal, date and time of saving, functional unit (intermediate or fuel), reaction type (electrochemical/thermochemical), CO2 conversion, whether standard utility demands were used (Gendorf), energy efficiency, benchmark process, benchmark scaling factor, use of avoided burden or allocation, user assumptions comment, totals of the contribution analysis result.

UpdateProcessAssumptions

Location: module – Worksheet_Maintenance

Updates the process assumptions text box at the top of the currently active sheet with the following information:

- Functional unit: fuel or chemical intermediate
- Benchmark process name and scaling factor or lack of benchmark process
- Stoichiometry-related data generation assumptions
    - Thermochemical, electrochemical, or average values selected by user for energy demand.
    - Brute reaction equation
    - Specified CO_2 conversion.
- Manual adaptation comment made by the user in the manual adaptation checkbox.

- Alert if non-characterized emissions occur in the process inventory.
- Alert and approach chosen for multifunctionality if by-products exist in the process inventory.

Calls *update_sb_overview* to update the system boundary overview next to the process assumptions text box.

update_sb_overview

Location: module – Worksheet_Maintenance

Updates the system boundary overview figure next to the process assumptions text box. The overview figure includes:

- process name,
- main product,
- whether waste streams occur,
- whether by-products occur, and, if so, which approach to multifunctionality is chosen.

A. Clear Functions

Clear functions empty specific parts of the active worksheet and are usually called from *Worksheet_Change* events.

Location of all clear commands: Modules: Worksheet_Maintenance

clear_bre

clear the gross reaction equation (*varBRE*) and also reset stoichiometric coefficient of main product to 1.

clear_min_energy_dem

clear minimum energy demand (*varMinEnergyDem*)

clear_act_energy_dem

clear actual energy demand (*varEnergyDem*)

clear_pi

clear the active *Process Inventory Table* (incl. all potentially pre-existing dropdown lists in the *"linked process"* column)

clear_allocation

clear *table_allocation*, as well as the allocation criterion and optionally added allocation comments. Additionally, uncheck *CheckBox_allocation* (leading to hiding *table_allocation*) and hide *CheckBox_allocation.*

clear_contrib_scen

for each *table_contrib_results* (sq, ld, hd, fd), clear everything but the header row and the first five columns of the Totals row;
also hide the textbox that potentially contains the information that the user declared substances as emissions for which environmental impacts are not characterized (*TFNotCharacterized)*;
also clear the amount of bound CO_2 in main and by-products (*varBoundCO2main* and *varBoundCO2byp*), and hide and clear the textbox *TFBoundCO2*

clear_tbl_current_ca

clear contents of *table_current_ca* (help table for contribution analysis figure)

clear_all_cats_contrib_results

clear results for process under study (i.e., columns 2 – 5) in *table_results_all_cats*

clear_all_cats_bm_impacts

clear results for benchmark process (i.e., columns 6 – 9) in *table_results_all_cats*

B. Variable name setter

setColumns

Location: Modules: TableColumnSetter

Assigns short-named variables to tables and columns in order to facilitate their usage in other code sections. setColumns is usually run on activation of Best-Case and Hotspot Assessment sheets. See the below figure for locations of the named tables on the sheet.

Tables located on Hotspot/Best-Case Assessment sheets:

- tbl_stoic **[1]**
  - col_stoic_substance
  - col_stoic_type
  - col_stoic_molFormula
- tbl_stoic_help **[2]**
  - col_stoic_molMass
  - col_stoic_hf
  - col_stoic_sf
  - col_stoic_coef
  - col_stoic_outputCoeffYield
- tbl_pi **[3]**
  - col_pi_ref
  - col_pi_amount
  - col_pi_unit
  - col_pi_type
  - col_pi_linpro
- tbl_allocation **[4]**
  - col_allocation_ref
  - col_allocation_type
  - col_allocation_factor

- tbl_contrib_results_sq **[5]**
  - col_contrib_results_sq_ref
  - col_contrib_results_sq_amount
  - col_contrib_results_sq_unit
  - col_contrib_results_sq_type

- tbl_contrib_results_ld **[6]**
  - col_contrib_results_ld_ref
  - col_contrib_results_ld_amount
  - col_contrib_results_ld_unit
  - col_contrib_results_ld_type

- tbl_contrib_results_hd **[7]**
  - col_contrib_results_hd_ref
  - col_contrib_results_hd_amount
  - col_contrib_results_hd_unit
  - col_contrib_results_hd_type

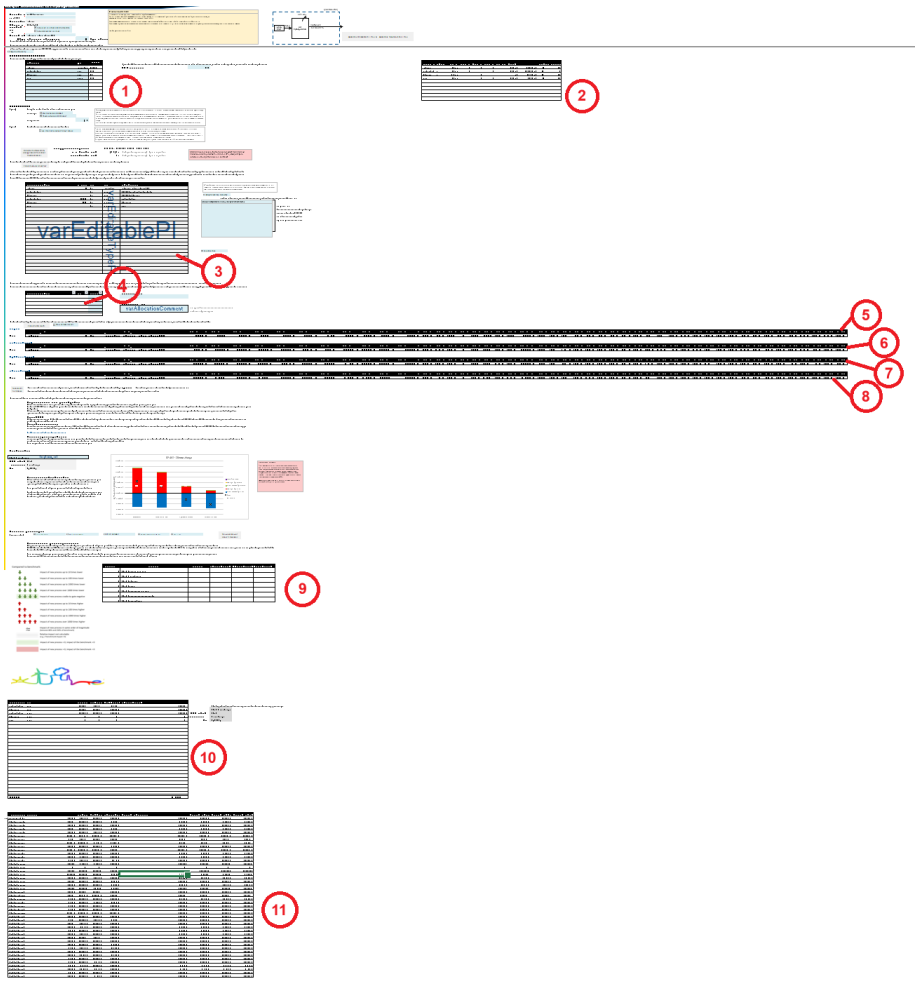
- tbl_contrib_results_fd **[8]**
  - col_contrib_results_fd_ref
  - col_contrib_results_fd_amount
  - col_contrib_results_fd_unit
  - col_contrib_results_fd_type

- contributionTables (1 To 4) [array containing all contribution tables]
- chart_ca [contribution analysis figure]

- tbl_rel_results_overview **[9]**
- tbl_current_ca **[10]**
  - col_current_ca_ref_prod
  - col_current_ca_type
  - col_current_ca_sq
  - col_current_ca_ld
  - col_current_ca_hd
  - col_current_ca_fd

- tbl_results_all_cats **[11]**
  - col_results_all_cats_bm_sq
  - col_results_all_cats_bm_ld
  - col_results_all_cats_bm_hd
  - col_results_all_cats_bm_fd

- benchmarkScenarioColumns (1 To 4) [array containing all benchmark scenario columns]



Tables that are NOT located on Hotspot/Best-Case Assessment sheets

- tbl_chemicals [on *chemicals* Worksheet, contains chemical properties]
  - col_chemicals_substance
  - col_chemicals_molForm
  - col_chemicals_molMass
  - col_chemicals_c
  - col_chemicals_h
  - col_chemicals_o
  - col_chemicals_s
  - col_chemicals_hf
  - col_chemicals_sf
  - col_chemicals_lhv
  - col_chemicals_conEcoPro
  - col_chemicals_isMix

- tbl_mix [on *New Mixture* Worksheet]
  - col_mix_substance
  - col_mix_wp
  - col_mix_mp

- tbl_mix_mean [on *New Mixture* Worksheet, contains the resulting properties]
  - col_mix_mean_value

- tbl_data_ei [on *data_ei* Worksheet, contains ecoinvent data]
  - col_data_ei_search

- tables on *scenario* sheet, contain scenario data for important products.
  - tbl_scen_co2
  - tbl_scen_hydrogen
  - tbl_scen_ng
  - tbl_scen_elec
  - tbl_scen_heat
  - tbl_scen_steam
  - scenarioTables (1 To 6) [array containing all scenario tables]

- tbl_data_own [on *data_own* Worksheet, contains data on self-created processes]

- tbl_impact_cats [on *impact categories* Worksheet, collection of all impact categories considered in ESTIMATe]

V. Mitigation Potential Assessment

Worksheet_Activate on MPA sheets

Location: MS Excel Objects – MPA_template and all copies

Once an MPA sheet is activated, the *MPA_Dropdown_Hotspot_Assessments* function is called to update the process choice dropdown menus at the top of the MPA sheet. After that, the active MPA sheet is protected.

Worksheet_Change on MPA sheets

Location: MS Excel Objects – MPA_template and all copies

- Check if two processes are chosen. If only one is chosen, give the other process a dummy name that will be recognized by all other functions so as not to break the sheet.
- If a process is chosen from the dropdown menu at the top of the MPA sheet
  - Check and terminate code if the same process is chosen twice
  - Check and terminate code if benchmark processes are not defined for both compared hotspot assessments.
  - Check and terminate code if LCA calculation has not been done for both compared hotspot assessments.

    - Clear all tables on the MPA sheet.
    - Copy inventory and result tables from the chosen hotspot assessment sheets
    - Adjust table headers to reflect the hotspot assessment names.
    - Copy the process assumptions of both compared hotspot assessments to the MPA sheet.
    - Update the shared resource dropdown below the process inventories.
    - Update the system boundary figures below the process inventory tables.
- If a shared resource is selected from the shared resource dropdown menu, enable the *scaling_start* button.
- If an impact category is selected from the impact category dropdown menu, Call *MPA_fill_current_ca_tables* and *MPA_merge_current_ca_tables* to update the tables *process1_current_ca*, *process2_current_ca*, and *current_ca*. Update the *chart_ca* accordingly by calling *MPA_Create_Chart*

MPA_Clear_Tables (sheetName as String)

Location: Module – MPA

Clears the following on the MPA sheet with the name *sheetName:*

- content of all tables
- process assumptions
- shared resource dropdown menu
- cells containing bound CO2 values and units
- *chart_ca*

MPA_Copy_Tables (shortname_process1 as String, shortname_process2 as String)

Location: Module – MPA

copies process inventory and contribution results tables from the Hotspot Assessment sheets *shortname_process1* and *shortname_process2* to the active MPA worksheet. If one sheetname is a dummy name, the tables are left empty.

Also sets the header information on main product, produced amount, unit, and benchmark process.

MPA_rename_table_headers (shortname1 As String, shortname2 As String)

Location: Module – MPA

adjust headers *of table_results_all_cats* and *system_boundaries* to include the process names *shortname1* and *shortname2.*

MPA_Edit_Tables (shortname_process as String, Processnumber as Integer)

Location: Module – MPA

Scales the inventory table and all results tables of the process *shortname_process* to a selected resource. *Processnumber* is either 1 or 2 and indicates whether current process is process1 or process2 on the active MPA sheet.

- Calls the *scalingFactor* function to determine the factor by which all tables need to be multiplied.
- Iterates over the *process_inventory* table's amount column and adjusts the value by multiplying with the scaling factor.
- Iterates over all *table_contrib_results* and multiplies all numeric values by the scaling factor.
- Adds a totals row to all *table_contrib_results.*
- Updates the amount of produced main product in the MPA sheet header.
- Calls *MPA_table_results_all_cats* to transfer the totals to *table_results_all_cats.*

MPA_fill_current_ca_tables

Location: Module – MPA

Fills the two tables *process1/2_current_ca* with the contribution analysis results for the impact category selected from the category dropdown menu.

MPA_merge_current_ca_tables

Location: Module – MPA

To make *chart_ca* easily understandable, this function merges the two tables *process1/2_current_ca* into one *table_current_ca* next to *chart_ca.* This allows the figure to display the same colors for, e.g., inputs shared between two processes.

The steps to merging are:

- Copy data from the *process1/2_current_ca* tables into *table_current_ca* at rows 1 and 28, respectively.
- Iterate through the rows from the bottom up, searching for matches in reference product and type for each row. If matches are found, merge the rows by adding up all values into one row and deleting the other.
- Sort the table by the "type" column.
- If by-products exist, add a row below *table_current_ca* indicating impacts without by-product credits.

MPA_make_colored_result_overview

Location: Modules: MPA

Compares the scaled environmental impacts of both assessed processes. The respective cells in *table_results_all_cats_compare* are colored in either yellow or blue.

- If **process 1** has a smaller environmental impact value than process 2 for impact category X (climate change, ozone depletion, …) and scenario Y (status quo, low-/high-/full-decarbonized), the corresponding comparison cell is colored **yellow.**
- If **process 2** has a smaller environmental impact value than process 1 for impact category X (climate change, ozone depletion, …) at scenario Y (status quo, low-/high-/full-decarbonized), the corresponding comparison cell is colored **blue.**
- CAUTION, there is ONE exception in the category: "ReCiPe Midpoint (H) V1.13 - Natural land transformation"
    - If **process 1** has a *higher* value for this impact category than process 2, the corresponding comparison cell is colored **yellow.**
    - If **process 2** has a *higher* value for this impact category than process 1, the corresponding comparison cell is colored **blue.**
- If both processes have the exact same environmental impact value for a certain impact category X at a certain scenario Y, the corresponding comparison cell remains transparent.

MPA_Dropdown_Hotspot_Assessments (sheetName as String)

Location: Module – MPA

Creates a list of existing Hotspot Assessment Sheets and creates the process choice dropdown menu at the top of the MPA sheet with the name *sheetName*. Hotspot assessment sheets are identified via a "1" in their respective A1 cell.

MPA_shared_resource_Dropdown (sheetName As String, shortname_process1 As String, shortname_process2 As String)

Location: Module – MPA

Creates a list of reference product/unit combinations shared between the two processes shortname*_process1* and *shortname_process2* on the MPA sheet named *sheetName.* Creates the shared resource dropdown menu.

The steps are:

- If one process is a dummy process (see Worksheet_Change for MPA), the code is terminated.
- The existing resource dropdown menu is deleted.
- The *commonresources* function is called to generate the list of reference product/unit combinations.
- The shared resource dropdown menu is created.
- If both processes have the same main product, the main product is preselected as the shared resource.

MPA_table_results_all_cats ()

Location: Module – MPA

Copies the impact totals of both compared processes in each scenario into the *_table_results_all_cats* located on the same MPA sheet.

MPA_Copy_Process_Assumptions (shortname_process1 As String, shortname_process2 As String)

Location: Module – MPA

Copies the process assumptions text box from the sheets named *shortname_process1* and *shortname_process2* to the active MPA sheet. Adjusts the title of each process assumptions box to reflect the process short name.
Also copies bound CO2 values to TFBoundCO2Info (still unscaled!)

MPA_system_boundaries_update (Processnumber As Integer)

Location: Module – MPA

Updates the flowsheet below the selection of the basis of comparison with process information (main product name, process name, benchmark) and highlights where in the process the basis of comparison is located using bold text. If no process is selected, the flowsheet is reset to default.

VI. Figures

fill_table_current_ca

Location: module – Figures

On Best-Case and Hotspot Assessment sheets. Fills *table_current_ca* with the reference products, types, and impacts in the currently selected impact category from the scenario results tables. The purpose is the easier creation and interpretation of the contribution analysis figure. Calls *clear_tbl_current_ca* before copying the data.

make_ca_figure

Location: module -Figures

Creates the contribution analysis (ca) stacked bar charts on Best-Case and Hotspot Assessment sheets based on the data in *table_current_ca*. Calls *fill_table_current_ca.* The benchmark is only shown in the chart if a benchmark process is chosen at the top of the assessment sheet. Totals without by-product credits are only shown in the chart if by-products exist within the assessment.

make_overview_figure

Location: module - Figures

Fills the visual overview table *table_rel_results_overview* with relative results first (new process divided by benchmark process) for all impact categories and scenarios. Then, sorts relative results into categories, each of which correspond to a picture indicated in the legend next to the overview figure. Finally, pastes pictures corresponding to the categories over each cell. Calls *make_pictures_hide_with_cells* and *show_selected_categories*.

make_pictures_hide_with_cells

Location: module – Figures

Defines all shapes whose name starts with “Picture” (and that are located on the active sheet) as part of their respective cell. This function needs to be run to hide the relative results overview images when rows (i.e., impact categories) are hidden. If this function did not exist, all pictures would be visible irrespective of whether their corresponding row is hidden.

delete_overview_figure

Location: module – Worksheet_Maintenance

clears both the images and the values entered in *table_rel_results_overview*. Identifies images to delete by their name starting with “Picture.”

show_selected_categories

Location: module – Figures

Hides all categories from *table_rel_results_overview* except for selected categories according to checkboxes above *table_rel_results_overview*. First, calls *make_pictures_hide_with_cells*. Then, determines row indices of rows to be hidden by comparing to properties on the impact categories sheet to the selected checkbox. Finally, hides entire rows according to indices determined in the previous step.

MPA_make_ca_figure

Location: module – MPA

Creates the contribution analysis (ca) stacked column figure on MPA sheets. In order to cluster columns together for each scenario, adds an empty column after every two columns. Totals without by-product credits are only shown if by-products exist.

Also creates Textbox containing the scaled values of and additional information on bound CO2 of main and by-products, if a “Climate change” impact category is selected to be shown in the ca figure.

MPA_show_selected_categories

Location: module – Figures

Similar to *show_selected_categories*, but on MPA sheets.

Hides all categories from *table_results_all_cats_compare and table_results_all_cats* except for selected categories according to checkboxes above *table_results_all_cats_compare. First,* determines row indices of rows to be hidden by comparing to properties on the impact categories sheet to the selected checkbox. Then hides entire rows according to indices determined in the previous step.

VII. Buttons and checkboxes on assessment templates

Buttons and checkboxes are located on all assessment sheets and templates if not specified otherwise.

Location: MS Excel Objects

A. Best Case and Hotspot Assessment calculation, in order of appearance

- **CheckBox_fuel_Click ():**
  - if True: user would like the main product of the assessment to be incinerated as a fuel.

- **CheckBox_intermediate_Click ():**
  - if True: user would like the main product of the assessment to be used as a chemical intermediate.

- **CheckBox_skip_stoic_Click ():**
  - Only on hotspot assessment sheets
  - If checkbox is checked, all calculation rows on top of the process inventory table are hidden (along with the checkboxes necessary to calculate the stoichiometry or process inventory).
    Therefore, the assessment is not based on stoichiometric calculations, and ESTIMATe expects manual process inventory entries.

- **CheckBox_Electro_Click ():**
  - if True: the energy demand for the process inventory is modeled as electricity input -> the Gibbs energy of the reaction is calculated.

- **CheckBox_Thermo_Click ():**
  - if True: the energy demand for the process inventory is modeled as heat input -> the enthalpy of the reaction is calculated.

- **CheckBox_Hischier_Gendorf_Click ():**
  - Only on hotspot assessment sheets
  - if True: due to poor data availability, the process inventory is built based on a standard approach with averaged ecoinvent utility amounts (for detailed information see the info box on the sheet of the current assessment)
    source: Hischier et al.[2]

- **Button_stoic_Click ():**
  - Calls *calculate_stoichiometry* which calculates stoichiometric reaction equation based on selected chemical input and output substances as well as previously set utility inputs, such as conversion rate and energy demand.

- **Button_process_inventory_Click ():**
  - Calls *calculate_process_inventory* which calculates and fills process inventory based on the stoichiometric reaction equation.

- **CheckBox_PI_manual_Click ():**

- Only on hotspot assessment sheets
- if True: process inventory can be manually changed, or entries added. the manual adaptations comment text box can be edited [**INFO**: *Enabled* is set to False, meaning that the manual adaptation of the process inventory cannot be deactivated anymore]
  if False: editing the process inventory and the manual adaptations comment text box is not allowed

- **CheckBox_allocation_Click ():**
  - Only on hotspot assessment sheets
  - if Checkbox "Use allocation" is checked, show table_allocation
    else: hide table_allocation.
  - Calls *UpdateProcessAssumptions*

- **Button_contrib_analysis_Click ():**
  - Calls *calculate_contribution_analysis* which calculates LCA results to fill contributionTables, creates LCA figure and compares LCA impacts to benchmark impacts.

- **CheckBox_ContribRes_Click ():**
  - if True: detailed LCA results in contributionTables are shown.

- **Button_save_to_own_Click ():**
  - Calls *add_to_data_own* which saves the LCA results to data_own sheet (that way the assessment can be utilized as a linked process for further assessments)

B. Mitigation Potential Assessment template

- **MPA_Scaling_start_Click ():**
  - Calls MPA_Edit_Tables to scale both compared hotspot assessments to the selected shared resource.
  - Calls MPA_fill_current_ca_tables and MPA_merge_current_ca_tables to update the tables *process1_current_ca*, *process2_current_ca*, and *current_ca.*
  - scales the bound CO2 values of the main product and by-products.
  - Calls *MPA_create_chart* and *MPA_make_colored_result_overview* to make contribution analysis and overview figures.
  - Calls *MPA_system_boundaries_update*

C. Figure creation and adaptation (all assessment templates)

Buttons and checkboxes for overview of impact categories

- **Button_ov_fig_Click ():**
  - updates and shows an overview of the impact categories that the user chooses to focus on (different options available, such as individual user selection that can be adjusted in the "impact category" sheet)
  - Calls make_overview_figure.

- **CheckBox_cats_showAll_Click ():**
    - if True: show LCA results for all impact categories.

- **CheckBox_cats_recipe_Click ():**
    - if True: show LCA results for ReCiPe impact categories.

- **CheckBox_cats_EF_Click ():**
    - if True: show LCA results for all EF impact categories.

- **CheckBox_cats_selection_Click ():**
    - if True: show LCA results for individually selected impact categories (individual selection can take place on the "impact categories" sheet)

- **CheckBox_cats_simpleEF_Click ():**
    - if True: show LCA results for reduced amount of EF impact categories.

VIII. Estimation methods

For individual descriptions of estimation methods including equation, source, and limitations, please refer to the *estimation methods* sheet in the ESTIMATe tool.

For each estimation method:

- Calculation Sub **[name of estimation method]_calc**
    - Location: module – estimation methods
    - Input parameters of the method are read and checked for completeness. For optional parameters, default values are used only if no user input for the parameter was made. If the user input for mandatory input parameters is incomplete, the calculation is terminated, and the user is asked to provide all necessary inputs.
    - Calculation according to equation specified in the box for the estimation method. Results are written to result cell.
- Button to start calculation **calc_[name of estimation method]_Click**
    - Location: worksheet – estimation methods
    - Starts the corresponding calculation sub.
- Button to jump back up to the overview table at the top of the page **met[index of method]_back_Click()**
    - Location: worksheet – estimation methods
- Information button **met[index of method]_information_button_Click()**
    - Location: worksheet – estimation methods
    - Shows information on the mandatory and optional input parameters in a popup window. The popup windows are Excel forms and called **met[index of method]_information**, respectively.

The overview table of estimation methods:

- Checkboxes for available input data in the overview table **CB_estim_met_ov_[parameter]_Click**
    - Location: Worksheet – estimation methods

    - On click on any checkbox, all corresponding row entries are colored in and the *Available_Methods* function is called to update the buttons under the overview table.
- Button to jump to method (from methods overview at top of page) **[name of estimation method]_Button_Click**
    - Location: worksheet – estimation methods
- **Available_Methods**
    - Location: Worksheet – estimation methods
    - For each estimation method, color in the corresponding button under the overview table if all required parameters are available, as indicated by a colored checkbox.

Worksheet_Change on *estimation methods* sheet

Location: Worksheet – estimation methods

- If input parameters for an estimation method change, reset the result of that estimation method.
- If entries are made in the "substance" or "wt.-%" column of *table_mean_properties,* the function *Table_mean_properties_Check* is called.

Table_mean_properties_Check

Location: Module – estimation methods

Calculates the average molar mass and specific heat capacity of all substances in *table_mean_properties,* weighted by the specified weight percentage. The function looks up values in the *chemicals* sheet except if the user specifies a value in *table_mean_properties*.

If the sum of weight percentages in *table_mean_properties* is larger than 1, the calculation is terminated, and the user is alerted.

Pumping_Piccinno_deltah

Location: Module – estimation methods

For the estimation method for pumping energy demands from Piccinno et al., an explicit calculation of the pumping height difference Δh is possible. This separate function reads the inputs for Δh, checks for completeness, and calculates Δh. A button to start this calculation, **calc_pumping_deltah_Click**, is located on the estimation methods sheet.

help_tables_Methods_Click

Location: Worksheet – estimation methods

Scrolls down to the table that calculates mean properties. **Jump_Back_3_Click,** located in the same location, scrolls back to the top of the worksheet.

IX. Helper Functions

Functions required for ESTIMATe and used throughout the code. Located in Module – Useful Functions if not indicated otherwise.

IsInArray

returns: Boolean
inputs: valToBeFound As Variant, arr As Variant

check if a value is in an array of values (developer: Ryan Wells wellsr.com)

lhvIsPositive

returns: Boolean
inputs: substance As String

checks if substance (most likely the main product) has a positive lower heating value in tbl_chemicals.

complementExists

returns: Boolean
inputs: component As Variant

GENDORF: (if INPUT is LIQUID and in chemicals a GASEOUS complement is also deposited) OR (if INPUT is GASEOUS and in chemicals a LIQUID complement is also deposited), 0.2 % of the all input materials are assumed to be emitted to air *(-> g);* the rest of all unreacted inputs (= all unreacted inputs - gaseous Complement) is assumed to be emitted to water *(-> l)*.

tableRowOfString

returns: Integer
inputs: str As String, col As ListColumn

returns the row number of a cell in a table (NOT the absolute row number of a cell in the sheet!)

tableRowOfStringWithAddress

returns: Integer
inputs: str As String, addr As String, col As ListColumn

returns the row number of a cell in a table (NOT the absolute row number of a cell in the sheet!)

selectTableInScenariosSheet

returns: ListObject
inputs: processname As String

Function selects the correct table in the *scenarios* sheet using the process name. To do so, the function compares the processname to the header of each scenario table. (Context: Each table on *scenarios* contains all four scenarios for one process)

areUnitsEqual

returns: Boolean
inputs: linkedProcessInPI As Range

goal: If the unit used in table_pi is the same unit as the one used in linked ESTIMATe/OWN/ecoinvent process, the function is True.
(linkedProcessInPI expected as Range of 1 Cell)

selectYellowCellsInRange

returns: nothing
inputs: searchRange As Range

all yellow cells in a range (commonly column) are selected, even if they are not connected.

enumerateInvalidAmounts

returns: String
inputs: colSubstance As ListColumn, colAmount As ListColumn

returns an enumeration of all PI substances whose set amounts are invalid (i.e., 0 or non-numerical)

enumerateInconsistentUnits

returns: String
inputs: colSubstance As ListColumn, colUnit As ListColumn

returns an enumeration of all PI substances whose set units do not match their specified ones (from linked ESTIMATe/OWN/ecoinvent process)

composeAllLinkedProcessErrors

returns: String
inputs: colType As ListColumn, colLinPro As ListColumn

returns all invalid linked processes (with the specific type: input/by-product/emission/waste) in one String as a preparation for a following message box

commonresources

returns: String
inputs: tbl_p1 As ListObject, tbl_p2 As ListObject

Compares the reference product columns of the two selected process inventories *tbl_p1* and *tbl_p2* for similarities to obtain a list of shared reference product/unit combinations. Only considers reference products of the types “by-product”, “main product”, and “input”. “Emission” and “waste” streams are not considered for common resources.

scalingFactorFunction

returns: Double
inputs: col_tbl_rp As ListColumn, col_tbl_unit As ListColumn, col_tbl_type As ListColumn, col_tbl_amount As ListColumn, sharedResource As String, MPA_Process_Name As String, Processnumber As Integer

calculates the scaling factor for an MPA process and also determines the system boundaries. The scaling factor describes the amount of main product produced from one unit of selected shared resource. Since the shared resource can occur simultaneously as two different types, e.g., as an input and main product simultaneously, the function further specifies which system boundary type the process represents.

There are four possible system boundaries that can occur as a result:

- Main Product → The shared resource is equivalent to the main product. The scaling factor equals 1 (no up-/downscaling of the process inventories necessary).
- Inputs/Outputs → The shared resource occurs both as input and output. The absolute difference between overall inputs and outputs equals the scaling factor.
- Inputs → The shared resource only occurs as input. The sum of all shared resource inputs equals the scaling factor.
- Outputs → The shared resource only occurs as output. The sum of all shared resource outputs equals the scaling factor.

The scaling factor calculation accounts only for *input, by-product, and main product* type reference products, since emissions and wastes cannot be selected as valuable shared resources. The code sums up the overall inputs (only *inputs* considered) and outputs (both *by-product* and *main product* considered) and returns the scaling factor as a decimal number. The system boundary of the process is entered to *tbl_system_boundaries*.

deleteLastMatrixColumn

returns: nothing
inputs: lin_ind_matrix () As Variant, actual_matrix () As Variant

function related to stoichiometric equation calculation. deletes the last column of both a) the matrix for checking linear independency (because it is a Zero-column) and b) the actual stoichiometric matrix.

switchMatrixColumns

returns: nothing
inputs: lin_ind_matrix () As Variant, actual_matrix() As Variant, colA As Integer, colB As Integer

function related to stoichiometric equation calculation. switches the position of two columns in both the matrix for linear independency check and the actual stoichiometric matrix (column pivoting)

lastOccRowOfCol

returns: Integer
inputs: letterOfColumn As String

finds the last occupied row of a column and returns its row index.

alignTextToShape

returns: nothing

inputs: sh As Shape

auto-size text to fit a text field.

- First: default font size in text field is set to 11 (if the text already fits into the text field, the font size will stay that way).
- While the text range is greater than the size of the text field, the font size is gradually reduced by 0.5pt until the text is properly aligned to the text field.
- To avoid too many steps in this While-Loop, the maximum number of repetitions is set to 50.

Button_scenFillRows_Click ()

Location: MS Excel Objects: scenarios

calls *fillRows* to fill the tables on the *scenario* sheet with impact data from the *data_ei* sheet (for data taken directly from the ecoinvent database)

fillRows

location: Worksheet – scenarios

some of the impacts of ESTIMATe scenario processes are provided directly from ecoinvent data:

- *ESTIMATe natural gas*: in "status quo" and "low-decarbonized" scenario, natural gas is provided by the current global natural gas mix (*ecoinvent*: "natural gas, high pressure, from market for natural gas, high pressure [RoW]").
- *ESTIMATe heat*: in "status quo" scenario, heat is supplied from natural gas combustions (*ecoinvent*: "heat, district or industrial, natural gas, from market for heat, district or industrial, natural gas [RoW]").
- *ESTIMATe steam*: steam is supplied by heat (according to *ESTIMATe heat*), an energy efficiency of 85% is considered for the vaporization of water.

protectWS

Location: Modules: Worksheet_Maintenance

input parameter: wsName As String

- activate Worksheet Protection on a Worksheet: every cell that is not highlighted in light-blue [RGB (218, 238, 243)] is locked and thus not editable as soon as worksheet protection is active.
- Best-Case Assessment sheets have more locked (and thus fewer editable) cells than Hotspot Assessment sheets.
- Background information: Cells are locked/unlocked by right clicking a cell, selecting "format cells" and then navigating to the "protection" tab, where the "locked" property can be set.
- Buttons and checkboxes are still usable.

additional protection settings:

- **Password: ="abcde"**
  password for unprotecting the worksheet
- **Drawing Objects:=True**
  protect shapes (text frames, figures etc.); charts are *excluded* from protection because their *"Locked"* checkbox is unchecked
- **Contents:=True**
  locked cells (i.e. all cells that do not have a light blue background) are protected
- **UserInterfaceOnly:=True**
  user interface is protected while macros are still allowed to run (even on locked cells)
- **AllowFormattingCells:=True**
  locked cells are not editable, but their format (bold text, background color etc.) can still be adjusted

The selection of protected and unprotected cells is allowed. Only the attempt to *edit* a locked cell (that does not include formatting the cell) will trigger a warning message.

unprotectWS

Location: Modules: Worksheet_Maintentance

input parameter: wsName As String

- deactivate Worksheet Protection on Worksheet with name wsName

Workbook_Open

Location: MS Excel Objects: ThisWorkbook

This function is called as soon as macros are enabled, **and** the ESTIMATe workbook is opened.

The *Overview* sheet is activated (as the entrance sheet). Subsequently, *ScreenUpdating* and *EnableEvents* are set to *True*.

General Error Handling (after every sub in which errors could occur)

```
'general error occurrence and handling
Postscript:
    Application.EnableEvents = True
    Call protectWS(ThisWorkbook.ActiveSheet.Name)
    MsgBox "An unspecified error has occurred while running." & vbNewLine & vbNewLine & _
           "Error Source: " & vbNewLine & Err.Source & vbNewLine & vbNewLine & _
           "Error Number: " & vbNewLine & Err.Number & vbNewLine & vbNewLine & _
           "Error Description: " & vbNewLine & Err.Description, _
           vbExclamation, "Unspecified error detected"
    Application.ScreenUpdating = True
```

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