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Supplementary information

EASETECH – an Environmental Assessment System for Environmental TECHnologies

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PART I: EXAMPLE OF TESTING OF THE CONCEPTUAL MODEL

The testing of the conceptual model was performed using the FitNesse Wiki, an automated testing tool which uses the Framework for Integrated Tests (Fit) to evaluate user stories in the context of the developed conceptual model. Figure S1 presents an example of such a Wiki page testing the correct computation of life cycle inventories (LCI).

This user story is one of the first ones that were implemented. It consists of 3 input tables and of one result table. The objective is to enter input values and check if the conceptual model gives the expected result in the last table. Note that the text outside of tables is only comments and is never evaluated.

In the 1st table, a waste process is defined that uses 2 MJ/kg of electricity per kg of wet weight of the input waste. This electricity is supplied by an external process called “1 MJ Electricity production (DK)”. The 2nd table describes the elementary flows induced by the external process “1 MJ Electricity production (DK)”: producing 1 MJ of electricity will emit 20 kg CO_2 into the air. The 3rd table describes the waste input: here the waste has a wet weight of 2 kg. Finally the last table computes the LCI of the process. The green color shows that the result is the one we expected: the emission of 80 kg of CO_2 into the air.

This simple example illustrates how basic calculations can be tested in the FitNesse Wiki.

We want to incinerate 2 tons of waste without any remains, and we are using 2 units per ton of the process "1MJ Electricity production (DK)".

WasteProcessFixture			
Amount	ExternalProcess	WasteProperty	edit?
-2 MJ/kg	1MJ Electricity production (DK)	Wet weight	true

ExternalProcessFixture			
Name	Flow produced	Amount	create?
1MJ Electricity production (DK)	"CO2, kg, to air"	20 kg/MJ	true

WasteFixture		
WasteProperty	Value	create?
Wet weight	2 kg	true

The result is a list of ElementaryFlow produced by the WasteProcess.

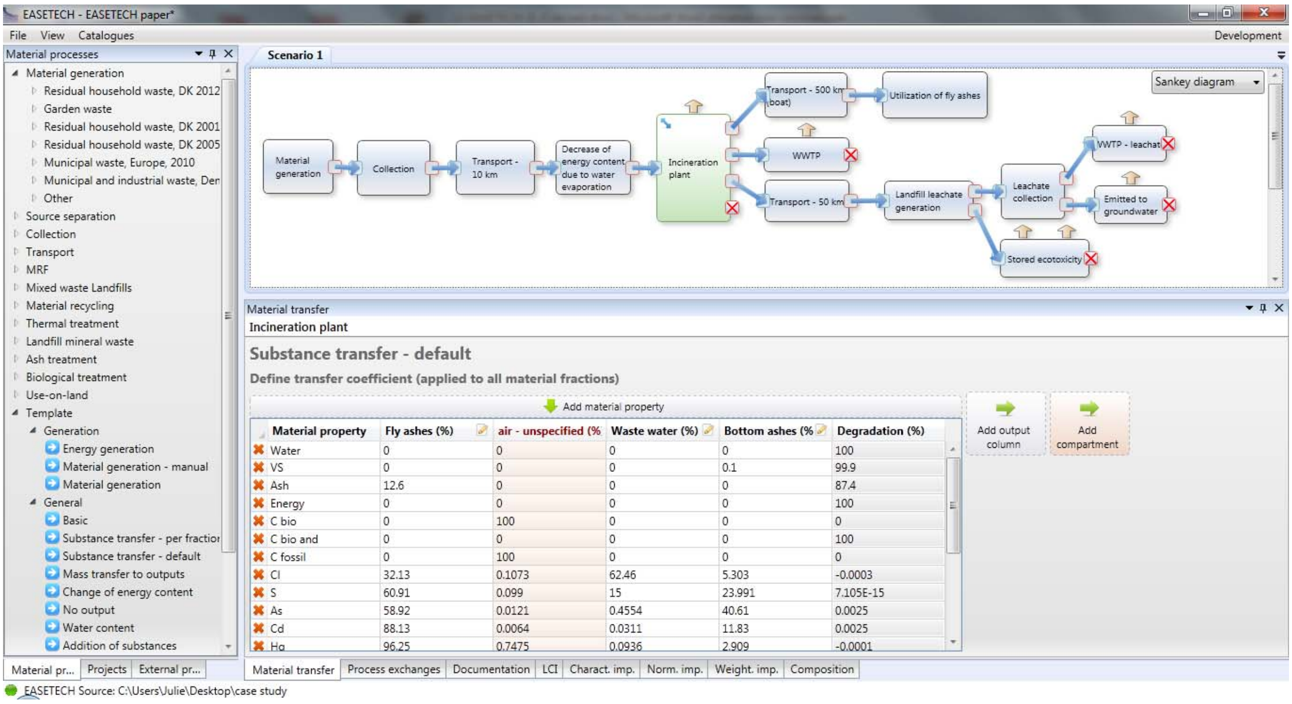
LciFixture	
ElementaryFlow	Amount
"CO2, kg, to air"	80 kg

Figure S1: Example of a FitNesse Wiki page testing the conceptual model

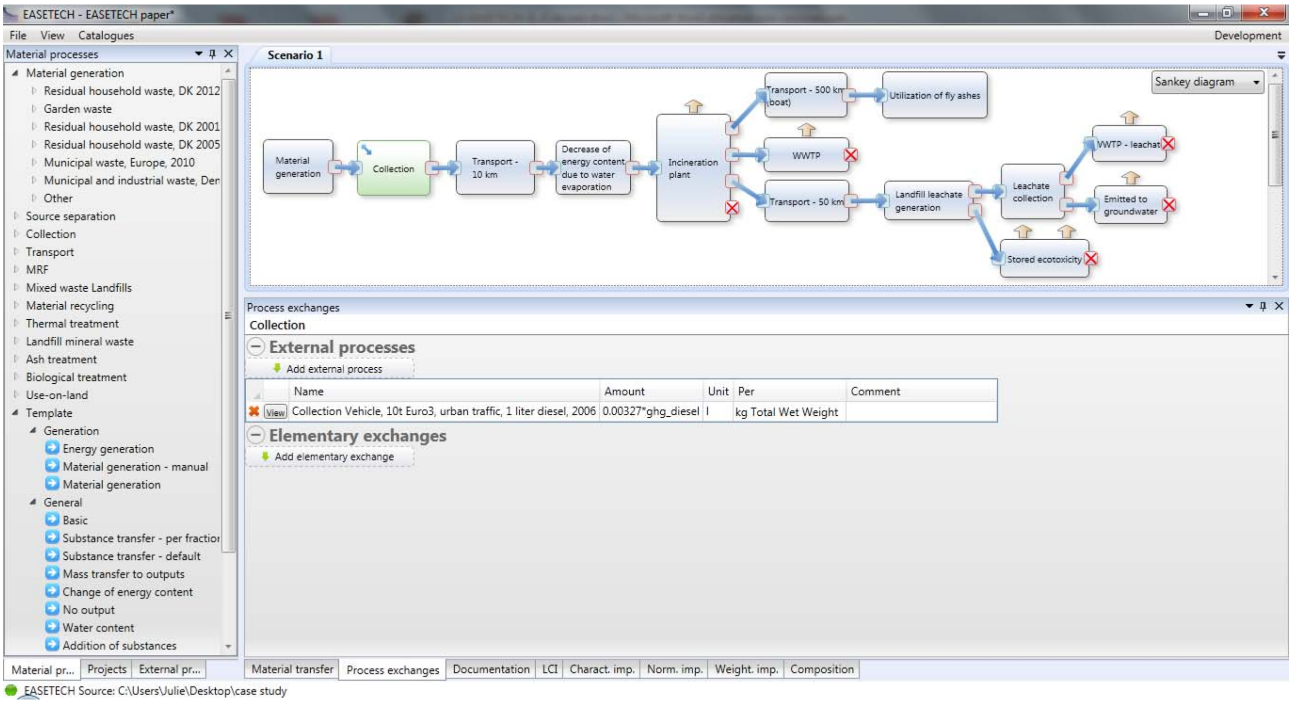
PART II: SCREENSHOTS

All numbers refer to the general overview of the interface in Figure 5 of the article.

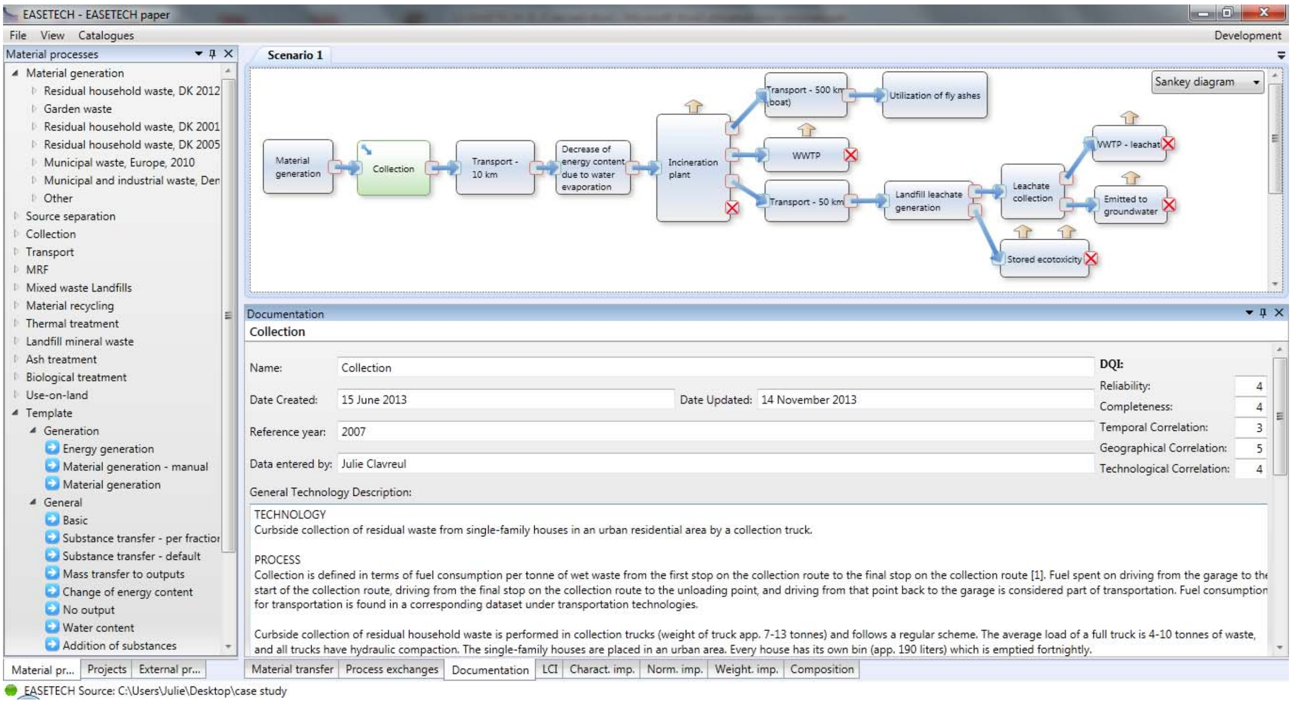
“Material transfer” tab (2a):



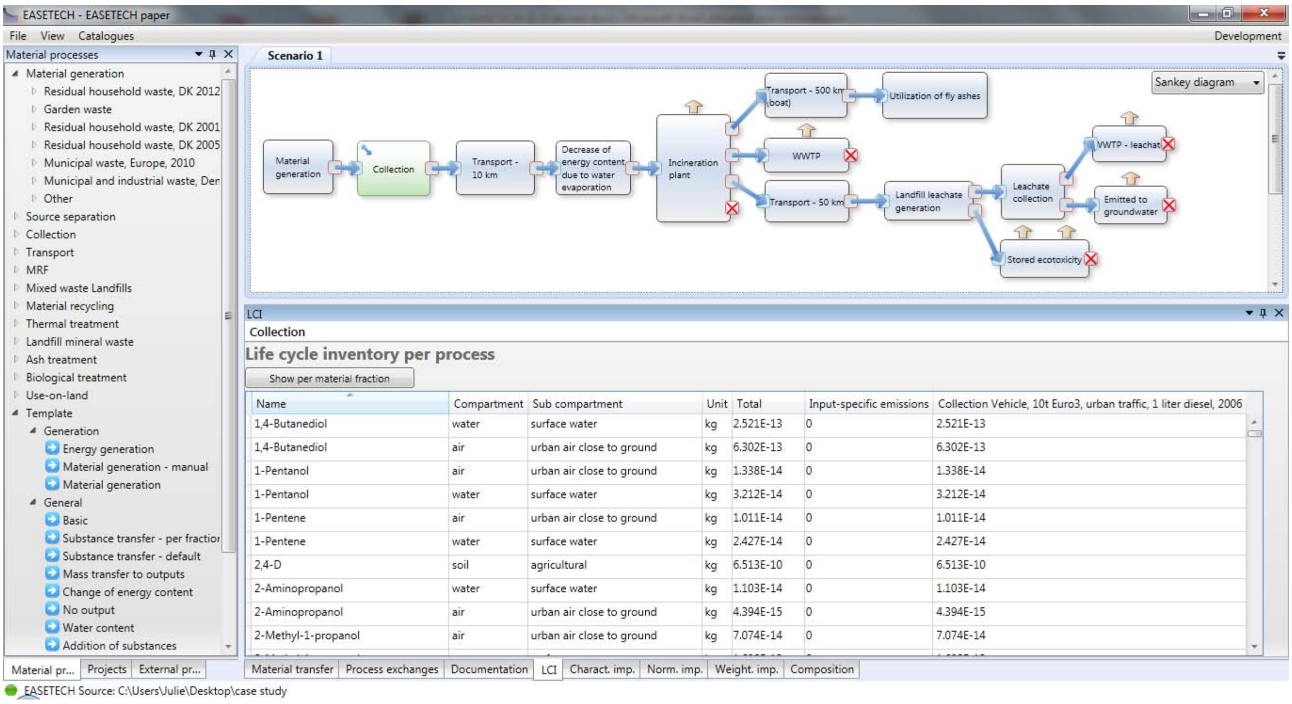
“Process exchanges” tab (2b):



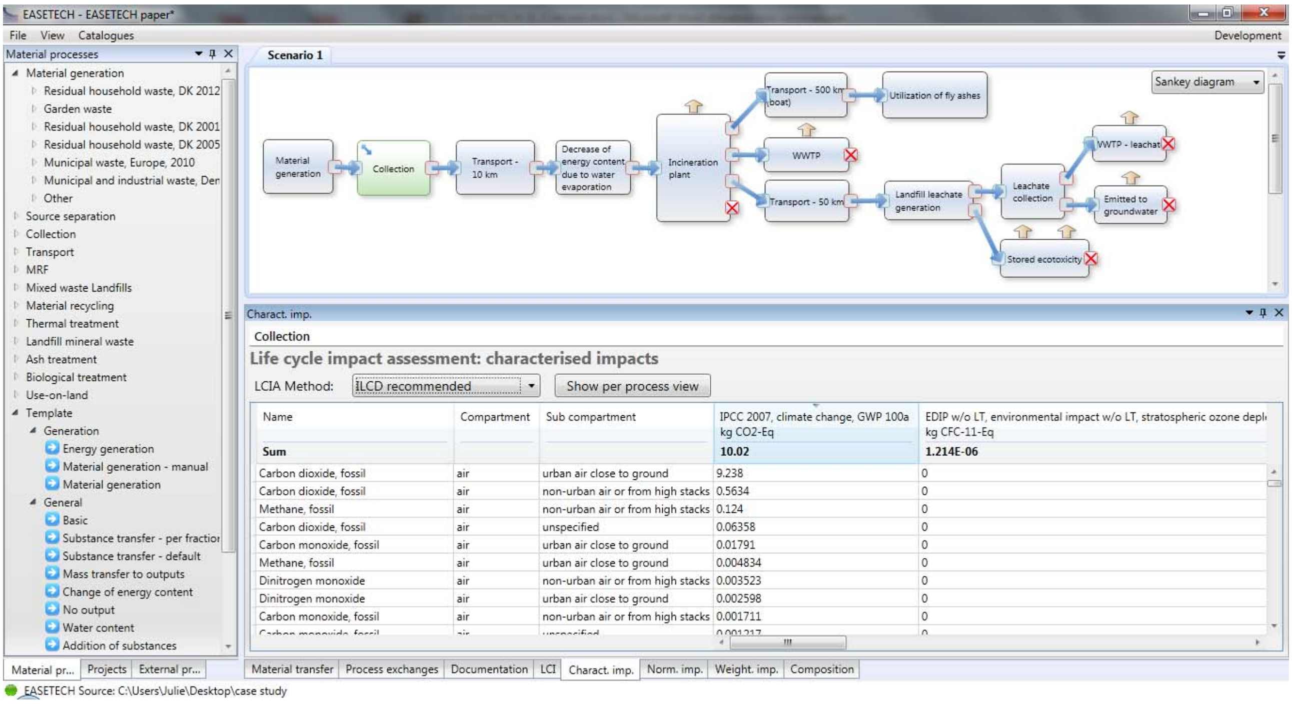
"Documentation" tab (2c):

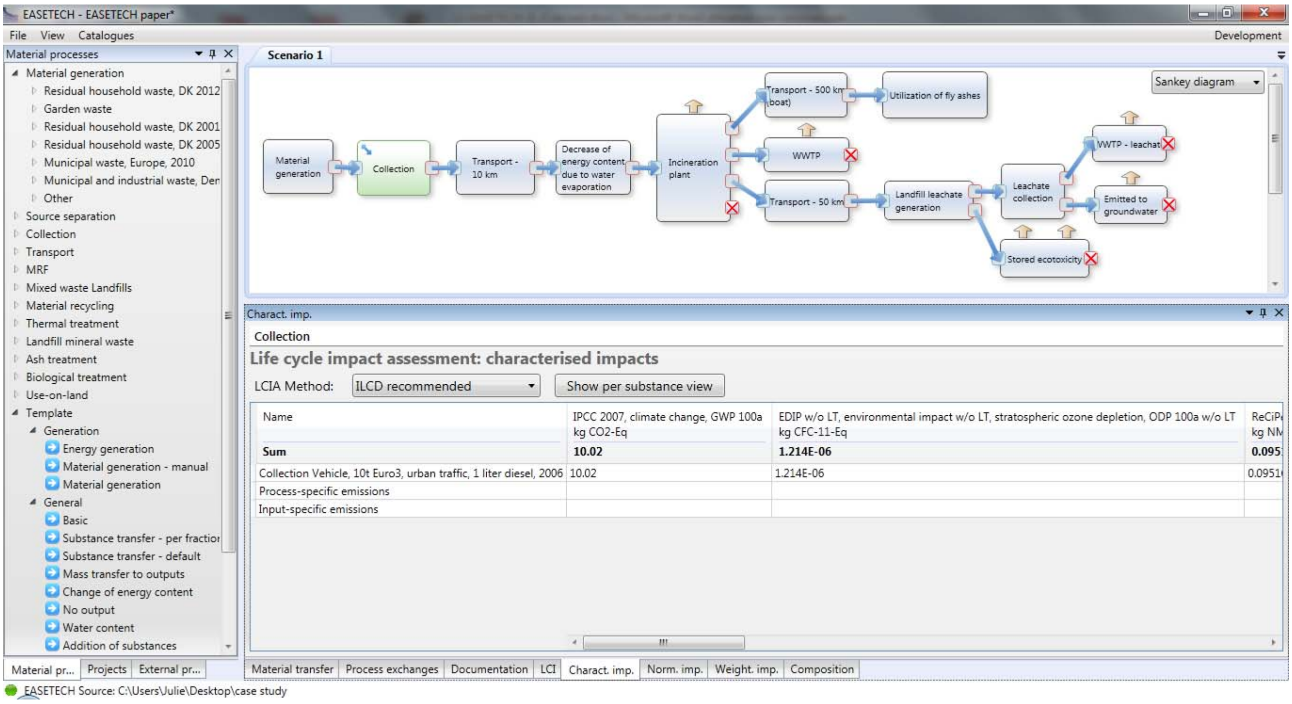


"LCI" tab (2d):

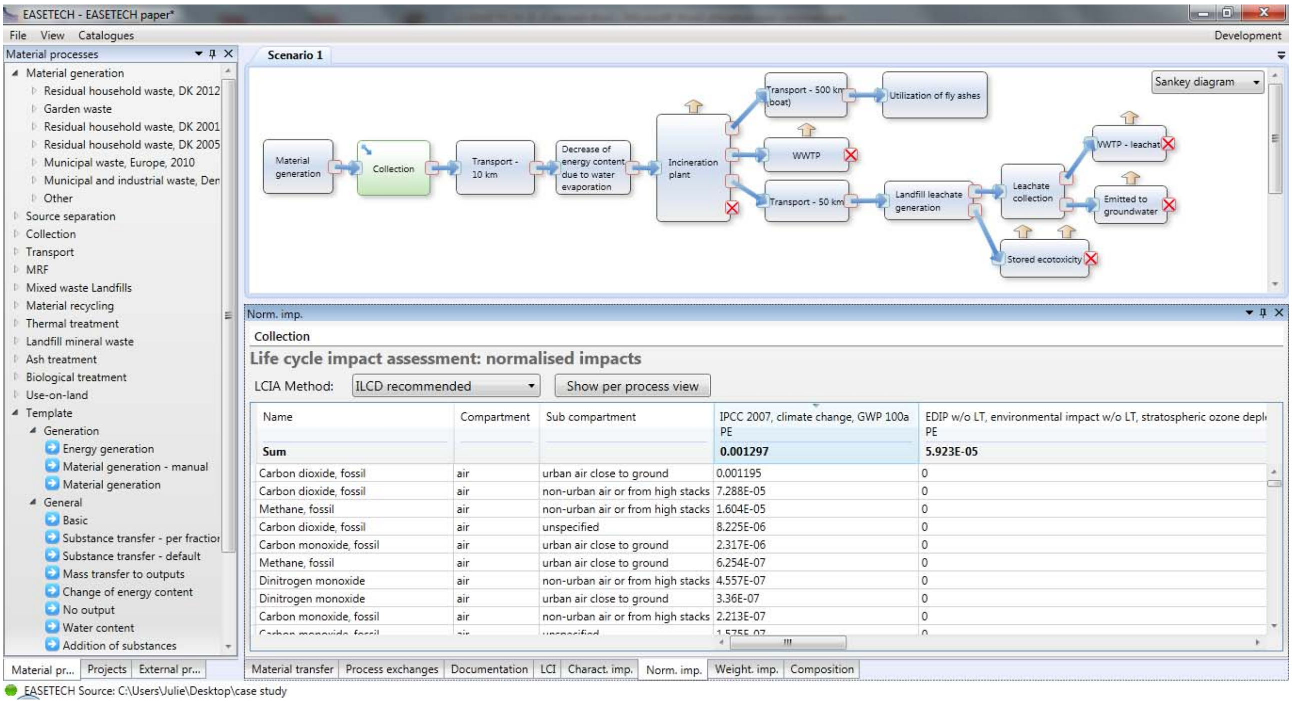


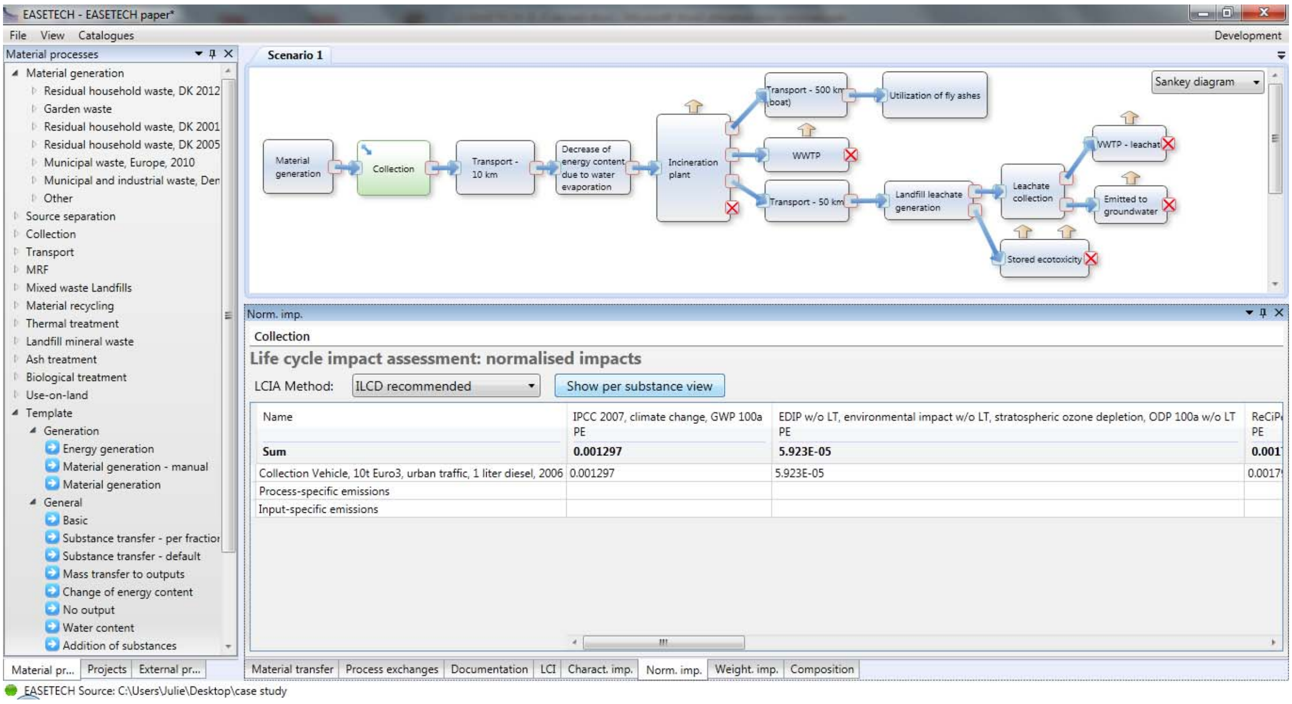
"Characterised impacts" tab, "per substance" and "per process" views (2e):



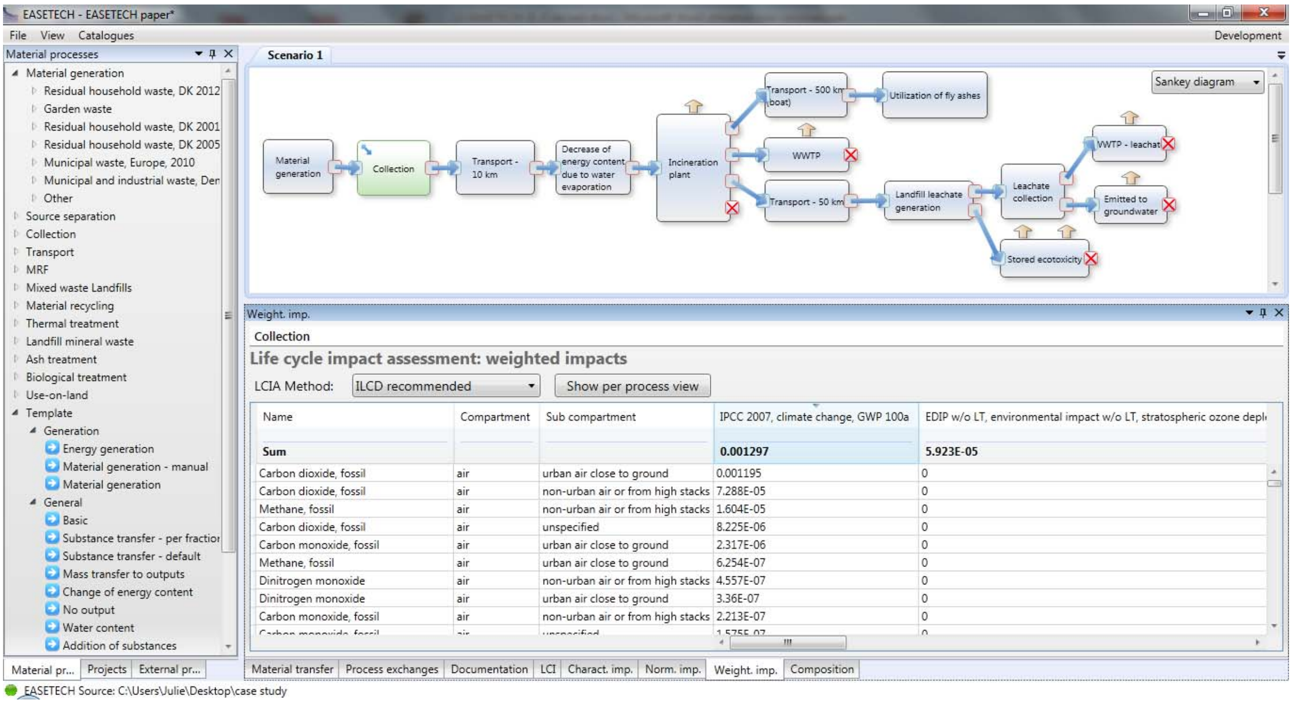


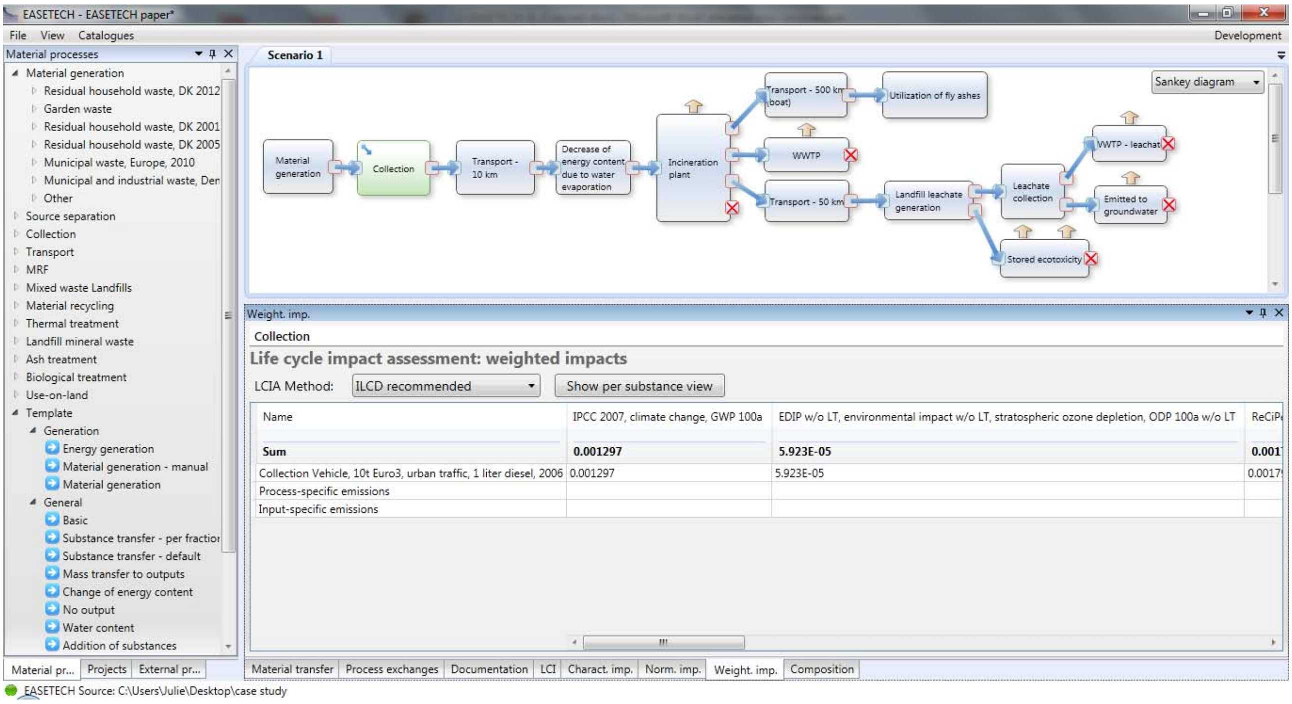
“Normalised impacts” tab, “per substance” and “per process” views (2f):



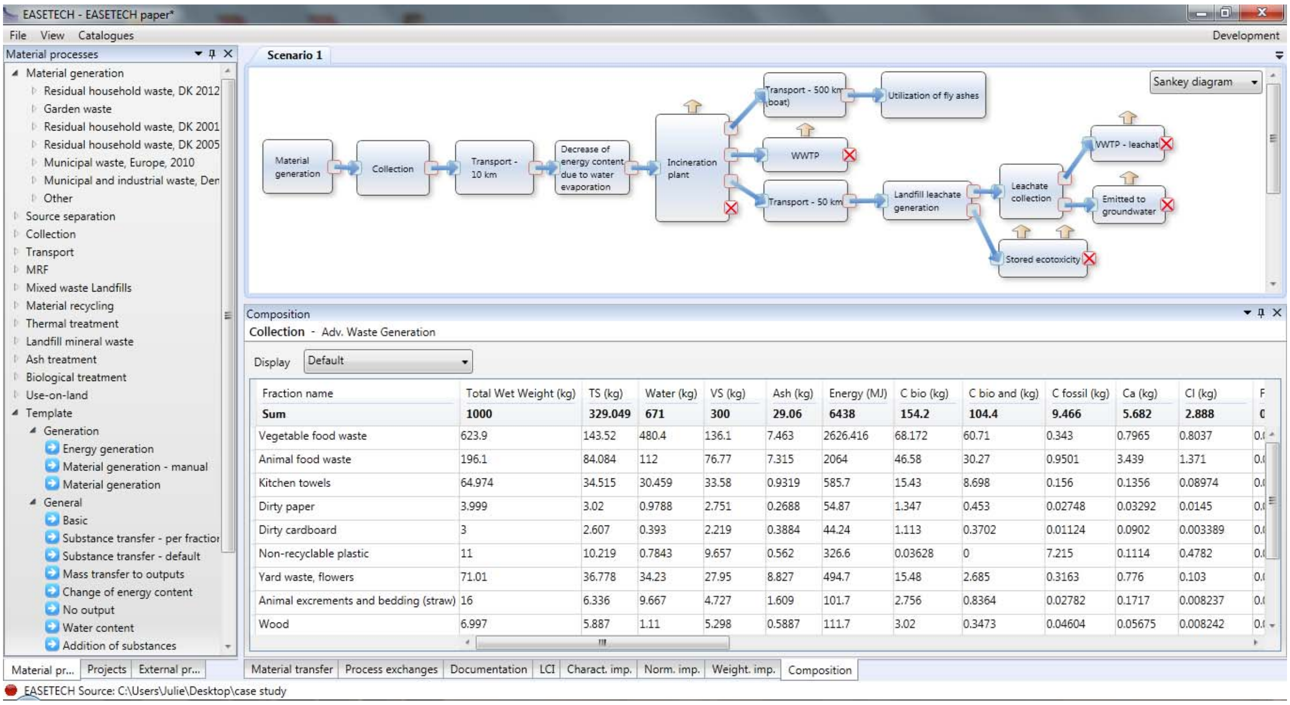


"Weighted impacts" tab, "per substance" and "per process" views (2g):

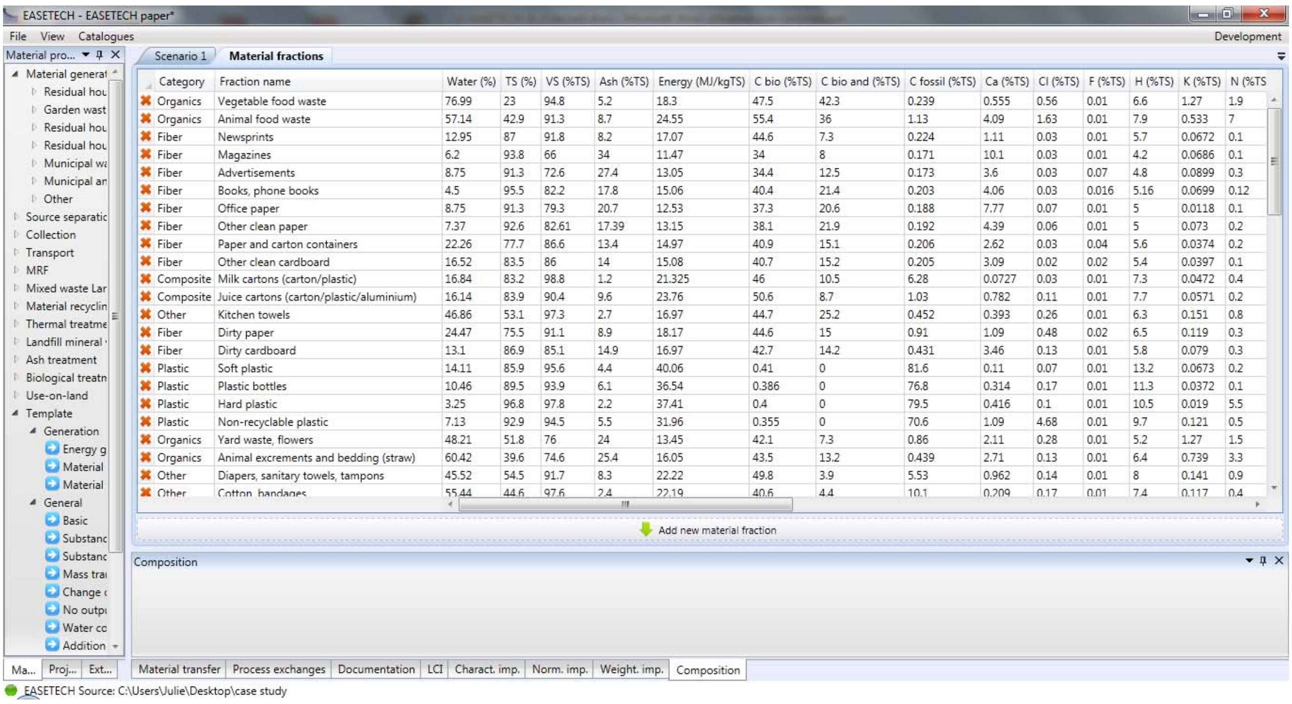




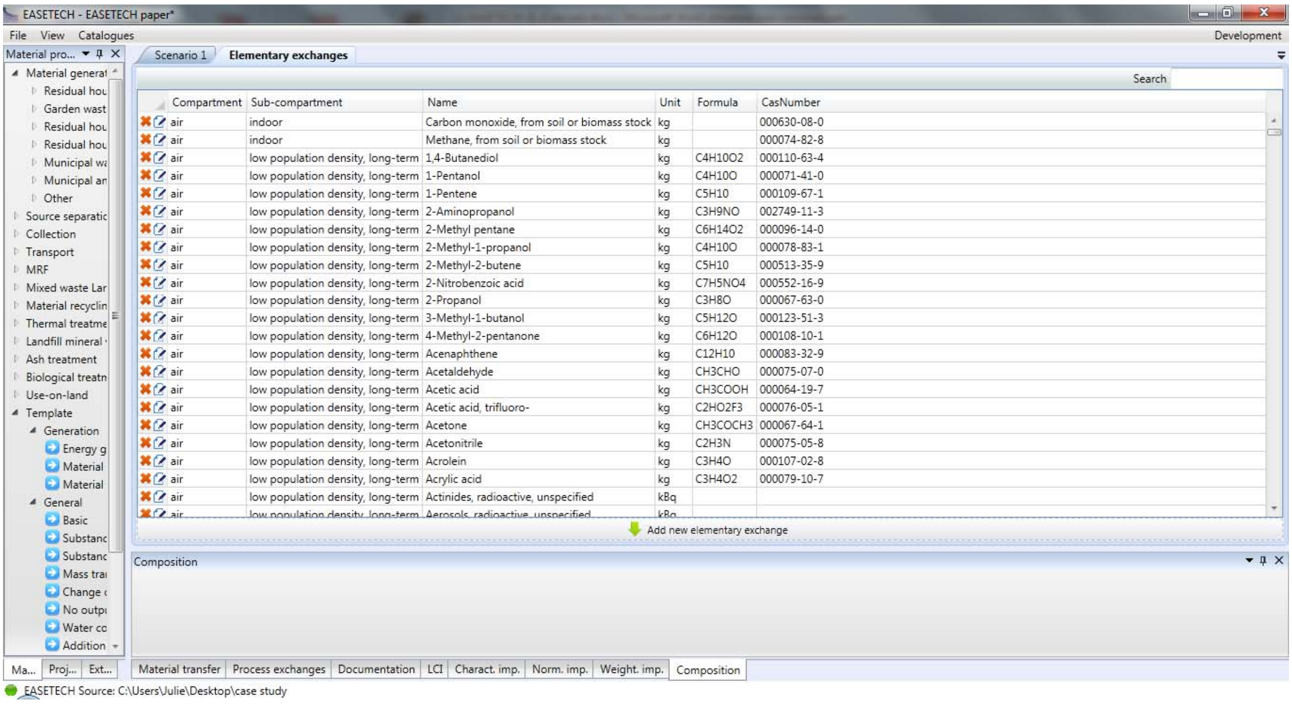
"Composition" tab (2h):



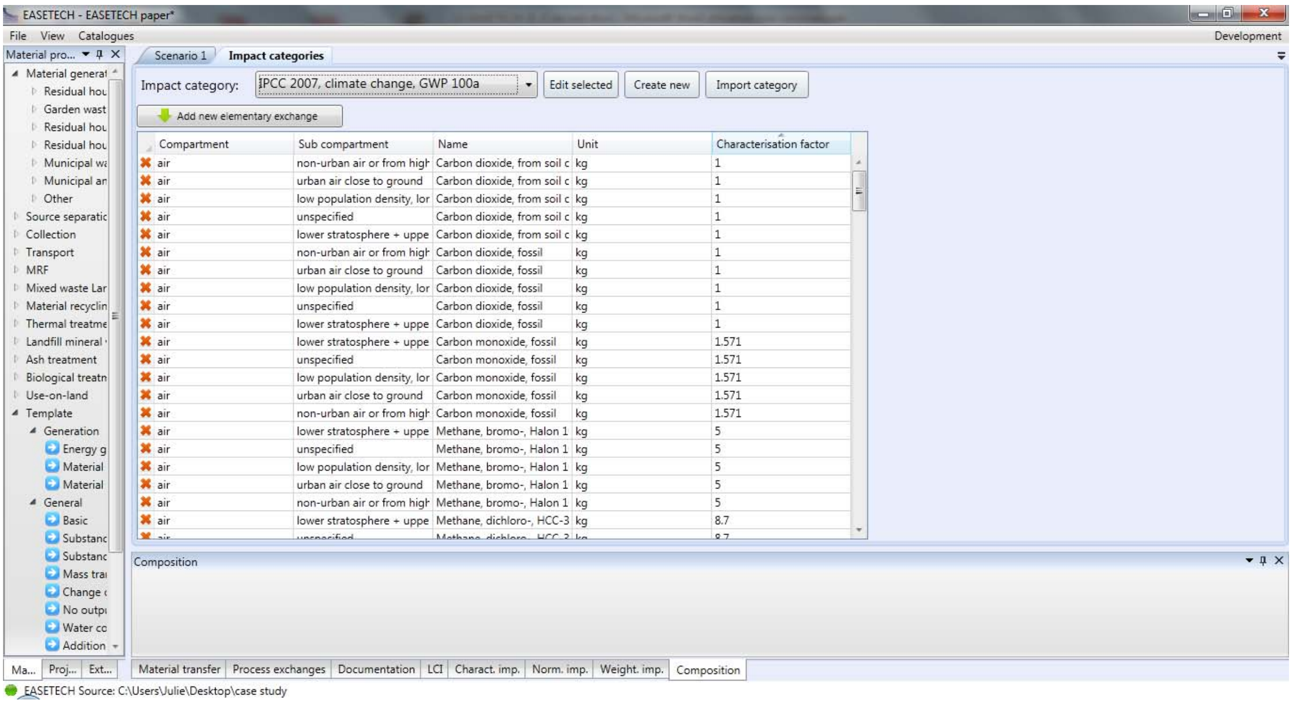
"Material fractions" catalogue (4a):



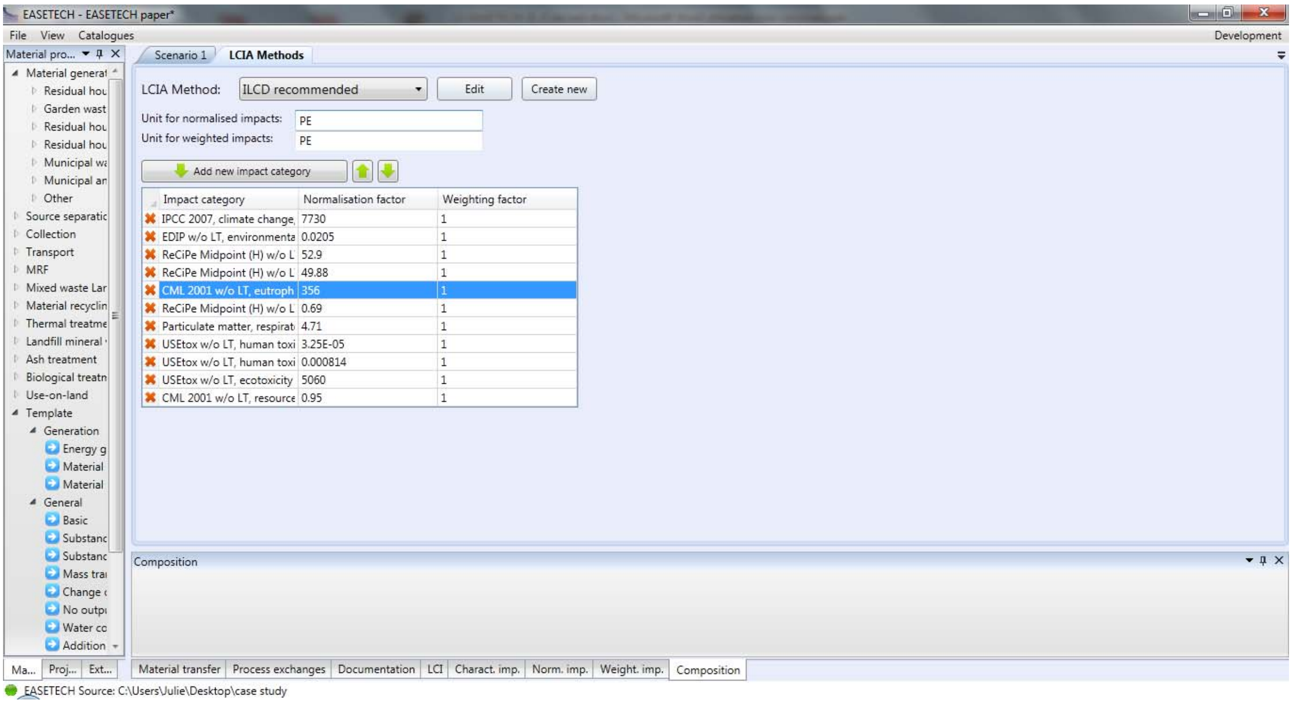
“Elementary exchanges” catalogue (4b):



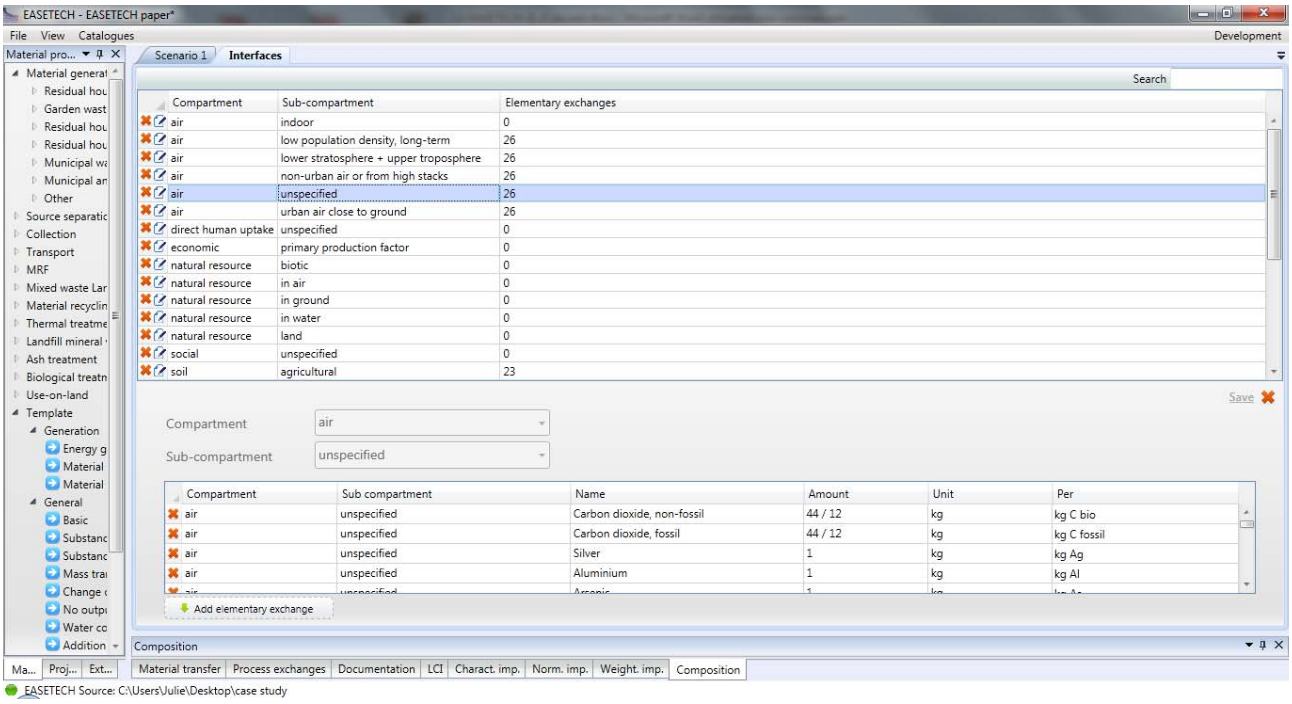
“Impact categories” catalogue (4c):



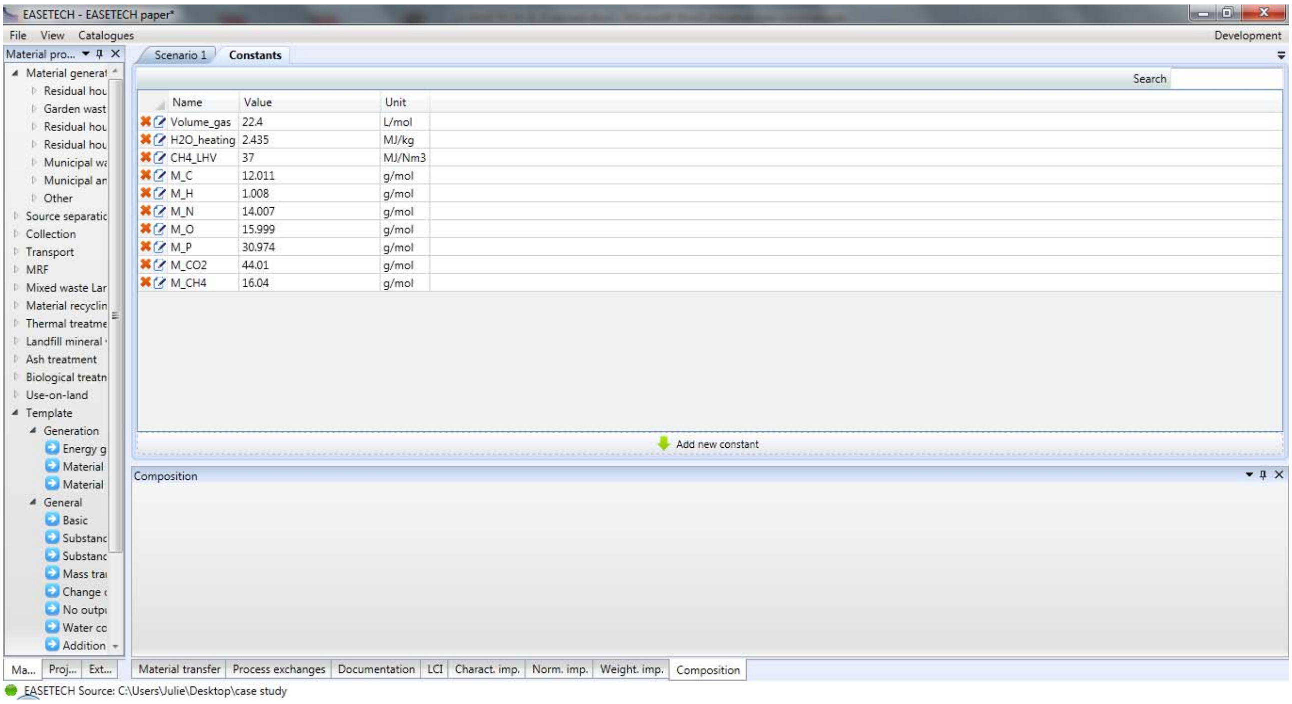
“Methods” catalogue (4d):



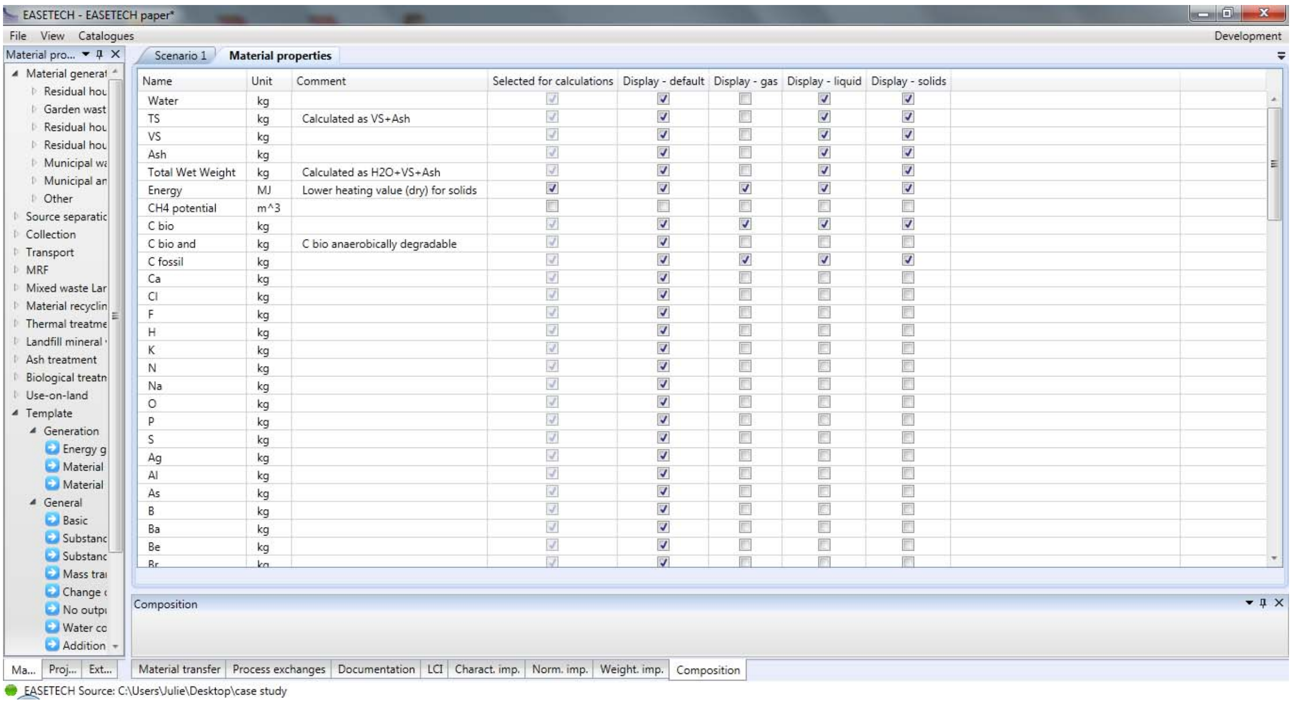
“Interfaces” catalogue (4e):



"Constants" catalogue (4f):



"Material properties" catalogue (4g):



PART III: DOCUMENTATION OF CALCULATIONS

This document was used to communicate with the development team and explain how calculations should be implemented. It uses simple words and lots of examples to illustrate the calculations happening in each template process.

In a first section, the different calculations of output flow compositions are presented. The second section describes the general LCA calculations happening in all processes, related to data in the "Process exchanges" tab, i.e. external processes and process-specific emissions. The third section presents the input-specific emissions calculated in 4 material processes whose "Material transfer" tab produces input-specific emissions.

1 Material composition calculations

1.1 Material generation

In this process, the user defines a TotalAmount and the composition in terms of fractions (called "percent" here). Data about each fraction are taken in the library of material fractions.

For each material fraction,

- water (kg) = water% (fraction)/100 *percent(fraction)/100 *TotalAmount (kg)
- vs(kg) = VS%(fraction))/100 * percent(fraction))/100 *TotalAmount(kg)
- ash(kg) = ash%(fraction))/100 * percent(fraction))/100 *TotalAmount(kg)
- energy (MJ) = energy%(fraction) * TS%(fraction)/100 *percent(fraction))/100 *TotalAmount(kg)
- for all other material properties: materialproperty(kg) = materialproperty%(fraction))/100 * TS%(fraction))/100 * percent(fraction))/100 *TotalAmount(kg)

where e.g. "ash%" is the ash content of the fraction in the library of material fractions.

Total wet weight and TS are calculated as usual, respectively as the sum of TS and water, and the sum of VS and ash. Figure S2 shows an example of material generation process.

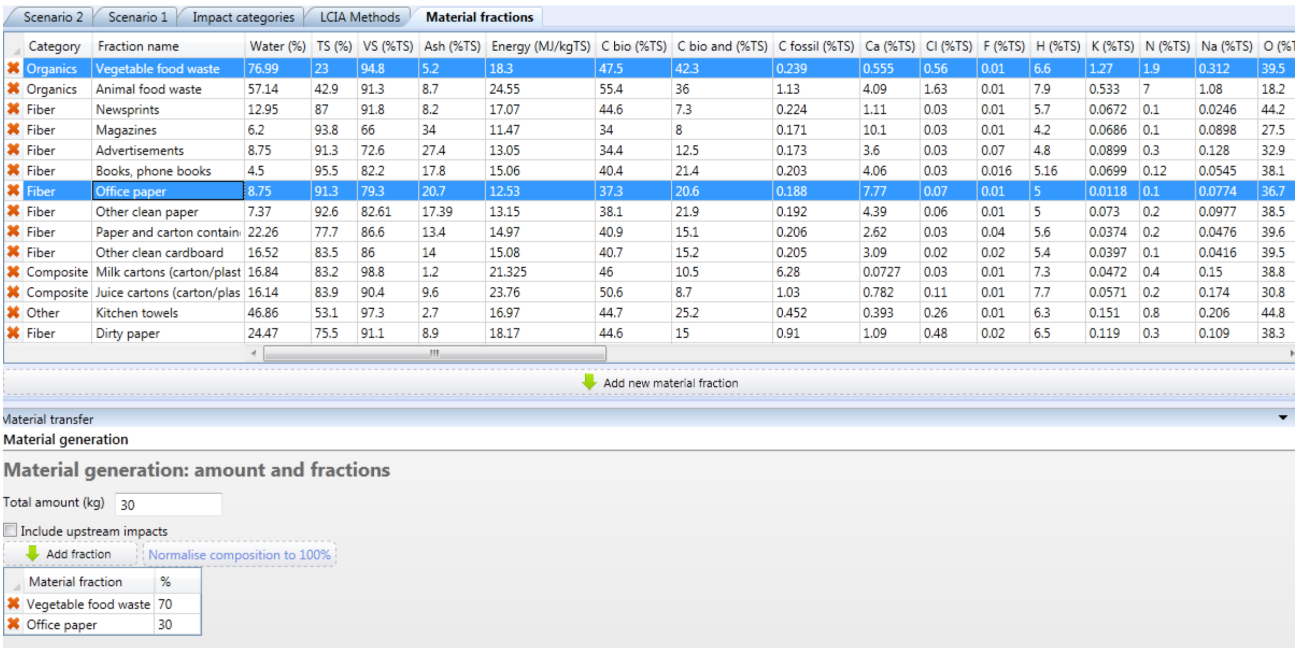
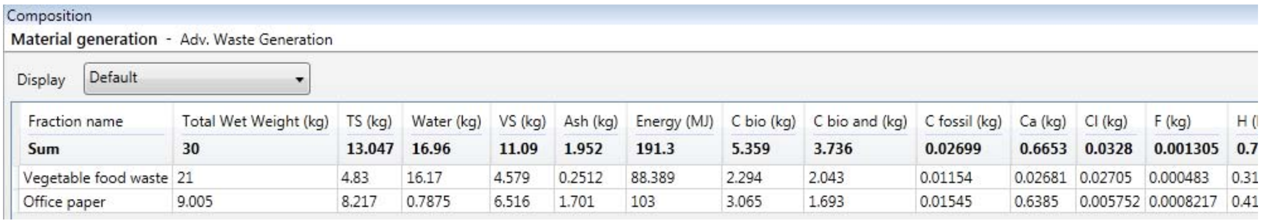


Figure S2: Material transfer of a "Material generation" process and catalogue of material fractions

The output is (Figure S3):

- for fraction “vegetable food waste”:
    - water: 76.99/100 * 70/100 * 30 kg = 16.169 kg
    - VS: 94.8/100*23/100*70/100*30 kg = 4.579 kg
    - ash: 5.2/100 *23/100 *70/100 *30 kg =0.251 kg
    - energy: 18.3*23/100*70/100*30 kg = 88.389 MJ
    - C bio: 47.5/100 *23/100 *70/100 *30 kg = 2.294 kg
    - ...
- for fraction “office paper”:
    - water: 8.75/100 * 30/100 * 30 kg = 0.7875 kg
    - VS: 79.3/100*91.3/100*30/100*30 kg = 6.516 kg
    - ash: 20.7/100 *91.3/100 *30/100 *30 kg =1.701 kg
    - energy: 12.53*91.3/100*30/100*30 kg = 102.96 MJ
    - C bio: 37.3/100 *91.3/100 *30/100 *30 kg = 3.065 kg


Composition
Material generation - Adv. Waste Generation
Display Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (
Sum	**30**	**13.047**	**16.96**	**11.09**	**1.952**	**191.3**	**5.359**	**3.736**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7**
Vegetable food waste	21	4.83	16.17	4.579	0.2512	88.389	2.294	2.043	0.01154	0.02681	0.02705	0.000483	0.31
Office paper	9.005	8.217	0.7875	6.516	1.701	103	3.065	1.693	0.01545	0.6385	0.005752	0.0008217	0.41

Figure S3: Material composition of the output of the “Material generation” process

1.2 Energy generation

The user defines a TotalAmount and the composition in terms of fractions (called “percent” here). Data about each fraction is taken in the library of material fractions.

For each material fraction,

- energy (MJ) = percent(fraction) /100 *TotalAmount(MJ)
- vs(kg) = VS%(fraction))/100 * percent(fraction))/100 *TotalAmount(MJ) /energy%(MJ/kg)
- ash(kg) = ash%(fraction))/100 * percent(fraction))/100 *TotalAmount(MJ) /energy%(MJ/kg)
- water (kg) = water%(fraction) / TS%(fraction) *percent(fraction)/100 *TotalAmount (MJ) /energy%(MJ/kg)
- for all other material properties: materialproperty(kg) = materialproperty%(fraction))/100 * percent(fraction))/100 *TotalAmount(MJ) / energy%(MJ/kg)

where e.g. “ash%” is the ash content of the fraction in the library of material fractions.

Total wet weight and TS are calculated as usual, respectively as the sum of TS and water, and the sum of VS and ash.

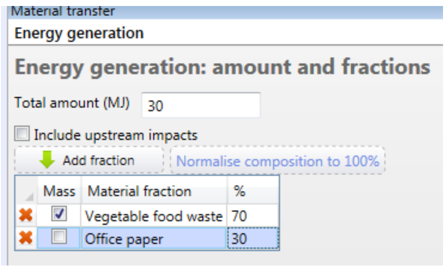


Figure S4: Material transfer of a “Material generation” process and catalogue of material fractions

Vegetable food waste is:

- Energy = 70/100 *30 MJ = 21 MJ
- TS = (70/100 *30 MJ) /18.3 MJ/kg = 1.148 kg
- VS = (70/100 *30 MJ) /18.3 MJ/kg *94.8/100 = 1.088 kg
- Ash = (70/100 *30 MJ) /18.3 MJ/kg *5.2/100 = 0.0597 kg
- Water = 76.99/23.01 *70/100*30 MJ /18.3 MJ/kg = 3.841 kg

Because the tickbox “Mass” is unticked for “Office paper”, this fraction has only:

- Energy = 30/100*30 MJ = 9 MJ


Composition
Energy generation - Adv. Energy Generation
Display Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)
Sum	**4.989**	**1.148**	**3.841**	**1.088**	**0.05967**	**30**	**0.5451**	**0.4854**	**0.002743**	**0.006369**	**0.006426**	**0.0001148**	**0.0757**
Vegetable food waste	4.989	1.148	3.841	1.088	0.05967	21	0.5451	0.4854	0.002743	0.006369	0.006426	0.0001148	0.0757
Office paper	0	0	0	0	0	9	0	0	0	0	0	0	0

Figure S5: Material composition of the output of the “Material generation” process

1.3 Material generation – manual

In this process, the user defines the number of fractions and the amounts of material properties directly. So the only thing to calculate is “Total solids (TS)” equal to VS+ash, and “Total wet weight (TWW)” equal to TS+waterContent.

1.4 Basic

Output = input.

1.5 Substance transfer per fraction

The number of outputs is determined by the user. The user can define the name of the output by right clicking on the column header in the table “Material transfer”. Each output has the same material fractions as the input (in terms of numbers and names).

For each output, for each fraction, for each material property,

outputNumber.fraction.property = input.fraction.property*TC(property, fraction, outputNumber)/100

where TC is a transfer coefficient input by the user in the table of “Material transfer” in an output column, in a material fraction line.

- If the fraction doesn’t exist in the table, the calculation uses the “default” line”.
- Also, by default, all TC are equal to zero in newly-created output columns.
- For each fraction line, the TC to the last output (called “Residues”) is defined as 100 minus the TC of the other columns, so when the other TC are not defined, 100% of the material property go to the output “Residues”.
- If a “degradation” output is added, a column “Degradation” is added which works like any other column, but a special cross-output is displayed and this output cannot be connected to any process. Note that only one degradation output can be created.

Example: For an input of 30 kg of 70% vegetable food waste and 30% office paper, we have the input flow specified in Table S1.

Table S1: Material composition of the input flow

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)	S (kg)	Ag (kg)	Al (kg)	As (kg)
Vegetable food waste	21	4.83	16.17	4.579	0.2512	88.389	2.294	2.043	0.01154	0.02681	0.02705	0.00483	0.3188	0.06134	0.09177	0.01507	1.908	0.01116	0.008887	0	0.004975	1.265E-06
Office paper	9.005	8.217	0.7875	6.516	1.701	103	3.065	1.693	0.01545	0.6385	0.005752	0.008217	0.4109	0.009696	0.08217	0.0636	3.016	0.003139	0.005284	0	0.1076	1.75E-06

We bring this to a “substance transfer per fraction” process with transfer coefficients specified only for VS and Hg:

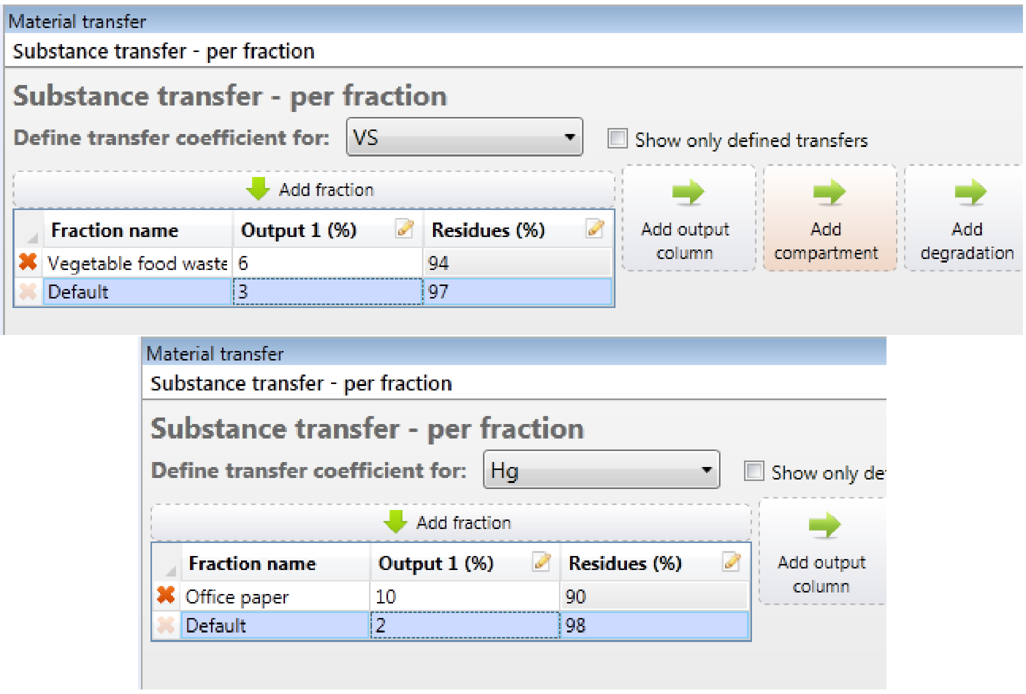


Figure S6: Material transfer for the “substance transfer per fraction” process

Output1 has:

- for fraction “vegetable food waste”:
  - VS: 4.579 kg * 6/100 = 0.275 kg
  - Hg: 9.66E-8 kg * 2/100 = 1.932 E-9 kg
  - all others: 0
- for fraction “office paper”:
  - VS: 6.516 kg * 3/100 = 0.195 kg
  - Hg: 2.925 E-7 kg * 10/100 = 2.925 E-8 kg
  - all others: 0

Output “residues” has:

- for fraction “vegetable food waste”:
  - VS: 4.579 kg * 94/100 = 4.304 kg

  - Hg: 9.66E-8 kg * 98/100 = 9.47 E-8 kg
  - all others equal to the fraction “vegetable food waste” in the input
- for fraction “office paper”:
  - VS: 6.516 kg * 97/100 = 6.321 kg
  - Hg: 2.925 E-7 kg * 90/100 = 2.632 E-7 kg
  - all others equal to the fraction “office paper” in the input

Composition

Substance transfer - per fraction - Output 1

Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)	S (kg)	Hg (kg)
Sum	**0.4702**	**0.4702**	**0**	**0.4702**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3.118E-08**
Vegetable food waste	0.2747	0.2747	0	0.2747	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.932E-09
Office paper	0.1955	0.1955	0	0.1955	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2.925E-08

Composition

Substance transfer - per fraction - Residues

Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)	S (kg)	Hg (kg)
Sum	**29.53**	**12.58**	**16.96**	**10.62**	**1.952**	**191.3**	**5.359**	**3.736**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**	**0.09999**	**0.02143**	**4.923**	**0.01147**	**0.01417**	**3.579E-07**
Vegetable food waste	20.72	4.555	16.17	4.304	0.2512	88.389	2.294	2.043	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134	0.09177	0.01507	1.908	0.01116	0.008887	9.467E-08
Office paper	8.809	8.022	0.7875	6.321	1.701	103	3.065	1.693	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696	0.008217	0.00636	3.016	0.0003139	0.005284	2.633E-07

Figure S7: Material composition of output1 and residues

1.6 Substance transfer default

This process is very similar to “substance transfer per fraction” except that it doesn’t allow the user to specify different TC for different material fractions. The number of outputs is determined by the user. The user can define the name of the output by right clicking on the column header in the table “Material transfer”. Each output has the same material fractions as the input (in terms of numbers and names).

For each output, for each fraction, for each material property,

outputNumber.fraction.property = input.fraction.property*TC(property, outputNumber)/100

where TC is a transfer coefficient input by the user in the table of “Material transfer” in an output column.

- It is the same transfer coefficients for all fractions.
- Also, by default, all TC are equal to zero in newly-created output columns.
- The default output is the “Degradation” output which cannot be removed and which cannot be connected to any process.
- The TC to the last output (called “Degradation”) is defined as 100 minus the TC of the other columns, so when the other TC are not defined, 100% of the material property go to the output “Degradation”.

The input composition is specified in Table S1 and this input is brought this to the “substance transfer default” process specified in Figure S8.

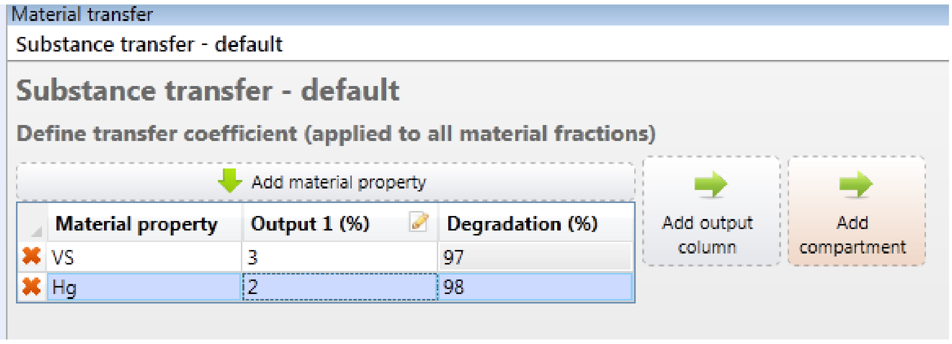
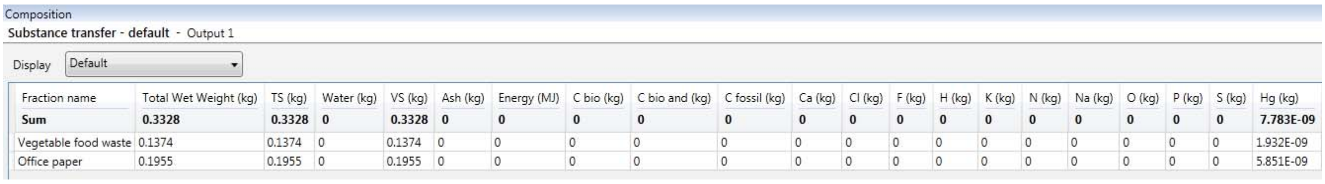


Figure S8: Material transfer for the "substance transfer default" process

Output1 has:

- for fraction "vegetable food waste":
  - VS: 4.579 kg* 3/100 = 0.137 kg
  - Hg: 9.66E-8 kg* 2/100 = 1.932 E-9 kg
  - all others: 0
- for fraction "office paper":
  - VS: 6.516 kg * 3/100 = 0.195 kg
  - Hg: 2.925 E-7 kg * 2/100 = 5.85 E-9 kg
  - all others: 0

And the output "Degradation" cannot be viewed.


Composition
Substance transfer - default - Output 1
Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)	S (kg)	Hg (kg)
Sum	**0.3328**	**0.3328**	**0**	**0.3328**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**7.783E-09**
Vegetable food waste	0.1374	0.1374	0	0.1374	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.932E-09
Office paper	0.1955	0.1955	0	0.1955	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.851E-09

Figure S9: Material composition of output1

1.7 Mass transfer to outputs

This process is similar to "substance transfer per fraction" but each output gets a transfer coefficient for the total mass, not specifically for each material property. The number of outputs is determined by the user. The user can define the name of the output by right clicking on the column header in the table "Material transfer". Each output has the same material fractions as the input (in terms of numbers and names).

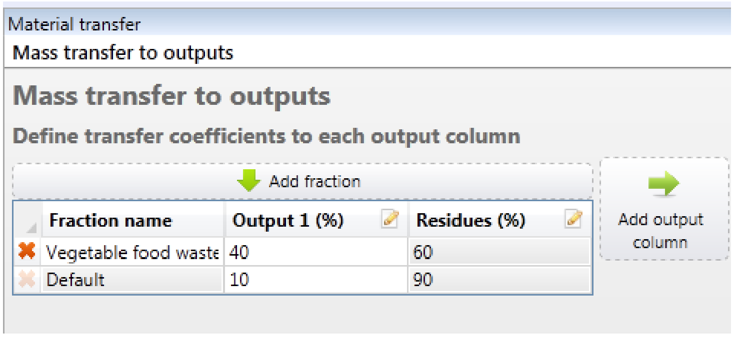
For each output, for each fraction, for each material property,

outputNumber.fraction.property = input.fraction.property*TC(fraction, outputNumber)/100

where TC is a transfer coefficient input by the user in the table of "Material transfer" in an output column, in a material fraction line.

- If the fraction doesn't exist in the table, the calculation uses the "default" line".
- Also, by default, all TC are equal to zero in newly-created output columnss.
- For each fraction line, the TC to the last output (called "Residues") is defined as 100 minus the TC of the other columns, so when the other TC are not defined, 100% of the material property go to the output "Residues".

The input composition is specified in Table S1 and this input is brought this to a "mass transfer" process with transfer coefficients specified in Figure S10.



Fraction name	Output 1 (%)	Residues (%)
Vegetable food waste	40	60
Default	10	90

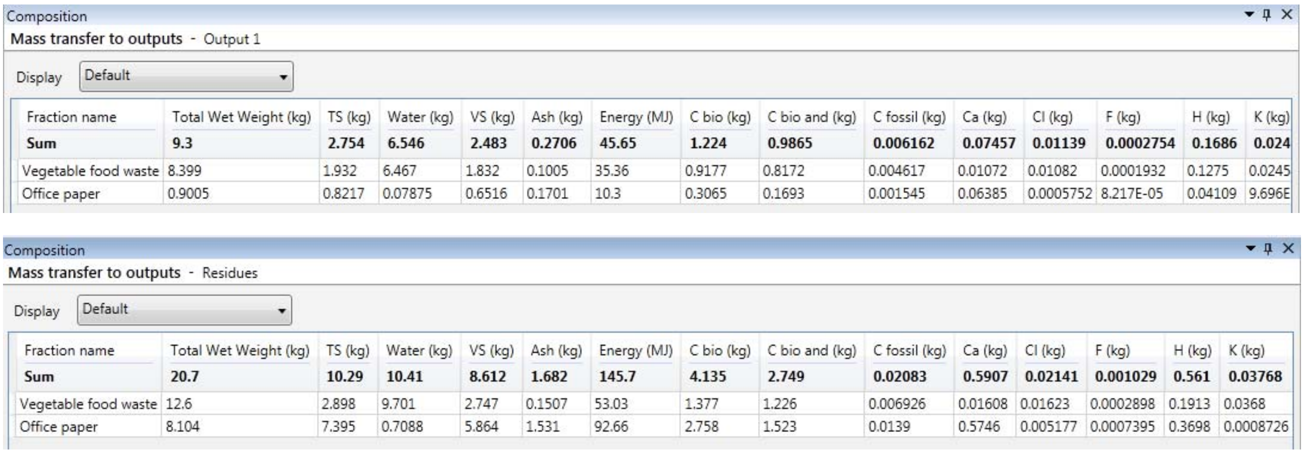
Figure S10: Material transfer for the "substance transfer default" process

Output1 has:

- for fraction "vegetable food waste": 40% of input of "vegetable food waste"
- for fraction "office paper": 10 % of input of "office paper".

Output "residues" has:

- for fraction "vegetable food waste": 60% of input of "vegetable food waste"
- for fraction "office paper": 90 % of input of "office paper".



Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)
Sum	**9.3**	**2.754**	**6.546**	**2.483**	**0.2706**	**45.65**	**1.224**	**0.9865**	**0.006162**	**0.07457**	**0.01139**	**0.0002754**	**0.1686**	**0.024**
Vegetable food waste	8.399	1.932	6.467	1.832	0.1005	35.36	0.9177	0.8172	0.004617	0.01072	0.01082	0.0001932	0.1275	0.0245
Office paper	0.9005	0.8217	0.07875	0.6516	0.1701	10.3	0.3065	0.1693	0.001545	0.06385	0.0005752	8.217E-05	0.04109	9.696E

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)
Sum	**20.7**	**10.29**	**10.41**	**8.612**	**1.682**	**145.7**	**4.135**	**2.749**	**0.02083**	**0.5907**	**0.02141**	**0.001029**	**0.561**	**0.03768**
Vegetable food waste	12.6	2.898	9.701	2.747	0.1507	53.03	1.377	1.226	0.006926	0.01608	0.01623	0.0002898	0.1913	0.0368
Office paper	8.104	7.395	0.7088	5.864	1.531	92.66	2.758	1.523	0.0139	0.5746	0.005177	0.0007395	0.3698	0.0008726

Figure S11: Material composition of output1 and residues

1.8 Change of energy content

There is one output with all material properties equal to the input, except for the output's energy content which is recalculated based on the following formula.

The principle is that the "energy content" is equal to the energy content of the input added to amounts depending on selected material properties. For example, the energy content is decreased of 2 MJ per kg of water content and decreased of 0.1 MJ per kg of Ash.

For each material fraction,

output.fraction.energycontent (MJ) = input.fraction.energycontent(MJ) + sumForAllProperties [value(fraction, slectedProperty)* input.fraction.selectedProperty]

where percent is the value given by the user between 0 and 100, which can be specified for each material fraction.

The input composition is specified in Table S1 and this input is brought this to a "change of energy content" process where the energy content is decreased of 3 MJ per kg of water content for all fraction except for "vegetable food waste" for which it is 2, and it is also decreased of 0.1 MJ per kg of Ash for all fractions.

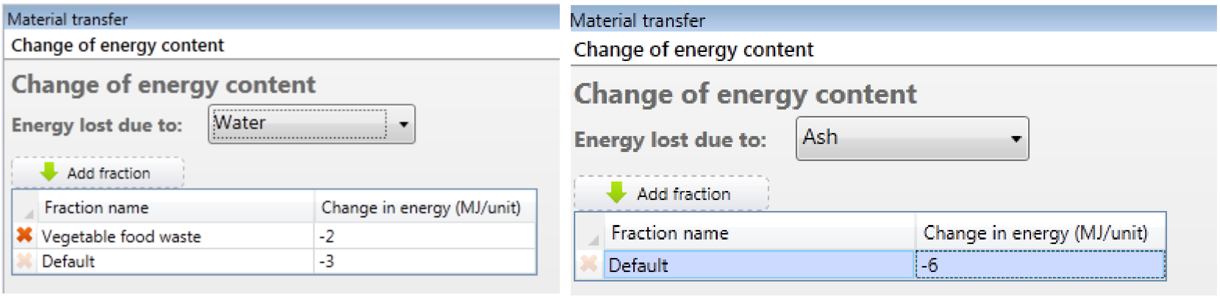
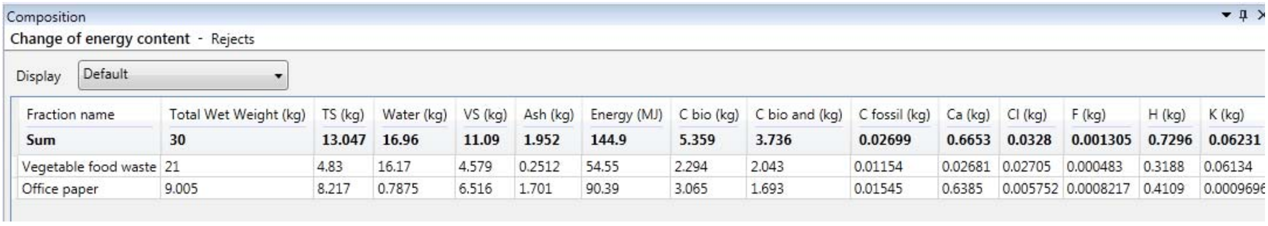


Figure S12: Material transfer of "Change of energy content"

So the calculation of the energy content is:

- for vegetable food waste, energycontent (kg) = energycontent (kg) + (-2)*water(kg) + (-0.1) *ash(kg) = 88.389 + (-2)*16.17 + (-6)*0.2512 = 54.54 MJ
- for office paper, energycontent (kg) = energycontent (kg) + (-3)*water(kg) + (-0.1) *ash(kg) = 103 + (-3)*0.7875 + (-6)*1.701 = 90.43 MJ



Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)
Sum	**30**	**13.047**	**16.96**	**11.09**	**1.952**	**144.9**	**5.359**	**3.736**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**
Vegetable food waste	21	4.83	16.17	4.579	0.2512	54.55	2.294	2.043	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134
Office paper	9.005	8.217	0.7875	6.516	1.701	90.39	3.065	1.693	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696

Figure S13: Material composition of the output

1.9 No output

No output.

1.10 Water content

There is one output with all material properties equal to the input, except for the output's water content which is recalculated based on the following formula.

For each material fraction,

output.fraction.water (kg) = input.fraction.TS (kg) * (percent(fraction) / (100-percent(fraction)))

where percent is the value given by the user between 0 and 100, which can be specified for each material fraction.

Of course the Total Wet Weight is changed, as it calculated as the sum of water and TS.

The input composition is specified in Table S1 and this input is brought this to a "water content" process and say that the water content should be 50% for vegetable food waste and 10% by default.

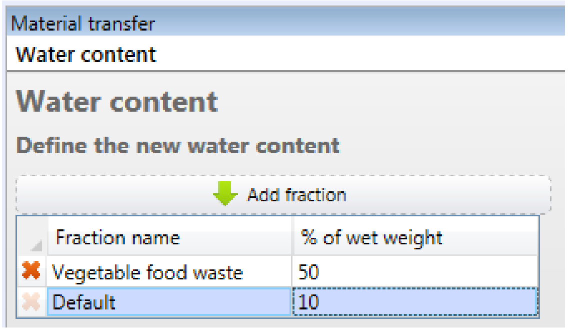
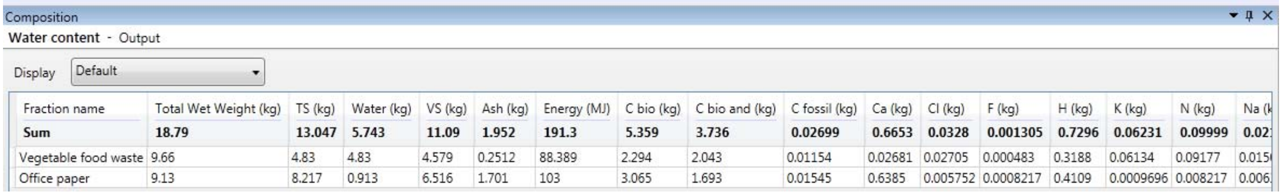


Figure S14: Material transfer of ”Water content”

So the calculation of the water content is:

- for vegetable food waste, water (kg) = TS (kg) * (50 /(100-50)) = 4.83 kg *(50/(100-50)) = 4.83 kg
- for office paper, water (kg) = TS (kg) * (10 / (100-10)) = 8.217 kg * (10 / (100-10)) = 0.913 kg


Composition
Water content - Output
Display Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (k
Sum	**18.79**	**13.047**	**5.743**	**11.09**	**1.952**	**191.3**	**5.359**	**3.736**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**	**0.09999**	**0.02**
Vegetable food waste	9.66	4.83	4.83	4.579	0.2512	88.389	2.294	2.043	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134	0.09177	0.015
Office paper	9.13	8.217	0.913	6.516	1.701	103	3.065	1.693	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696	0.008217	0.006

Figure S15: Material composition of the output

1.11 Addition of substances

There is one output with all material properties equal to the input, except for the material properties selected in the table of Material transfer. The calculations depend on which radio button has been selected by the user.

For each material property in the table, for each material fraction,

- if “solid material”:

output.fraction.selectedMaterialProperty = input.fraction.selectedMaterialProperty + amount(selectedMaterialProperty)*input.fraction.TotalWetWeight /10^6

- if “gas”:

output.fraction.selectedMaterialProperty = input.fraction.selectedMaterialProperty + amount(selectedMaterialProperty)* (input.fraction.ch4 + input.fraction.co2) /10^3

- if “liquid”:

output.fraction.selectedMaterialProperty = input.fraction.selectedMaterialProperty + amount(selectedMaterialProperty)*input.fraction.WaterContent /10^6

- if “energy”:

output.fraction.selectedMaterialProperty = input.fraction.selectedMaterialProperty + amount(selectedMaterialProperty)*input.fraction.EnergyContent /10^3

where “amount” is the value given by the user in the table, for the specific material property.

The input composition is specified in Table S1 and this input is brought this to a “addition of substances” process with in the table “Hg; 2”.

➢ **<u>If we select “solid”:</u>**

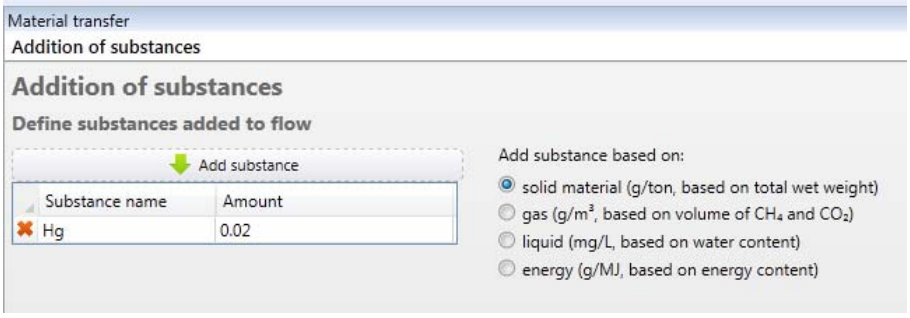


Figure S16: Material transfer of “Addition of substance” in the case of “solid” selection

The output is the same as the input except for Hg, which is:

- for vegetable food waste: 9.66E-8 kg + 0.02 g /10^6 g *21kg = 0.966E-7 kg + 4.2E-7 kg = 5.16E-7 kg.

- for office paper: 2.925E-7 kg + 0.02 g/10^6 g *9.005 kg = 2.925 E-7 kg + 1.801E-7 kg = 4.726 E-7 kg.

➢ **<u>If we select “gas”:</u>**

The output is the same as the input including for Hg as CO2 and CH4 are zero. To see the calculation, we add an anaerobic digestion process with yield of 10 % for all fractions (Figure S17).

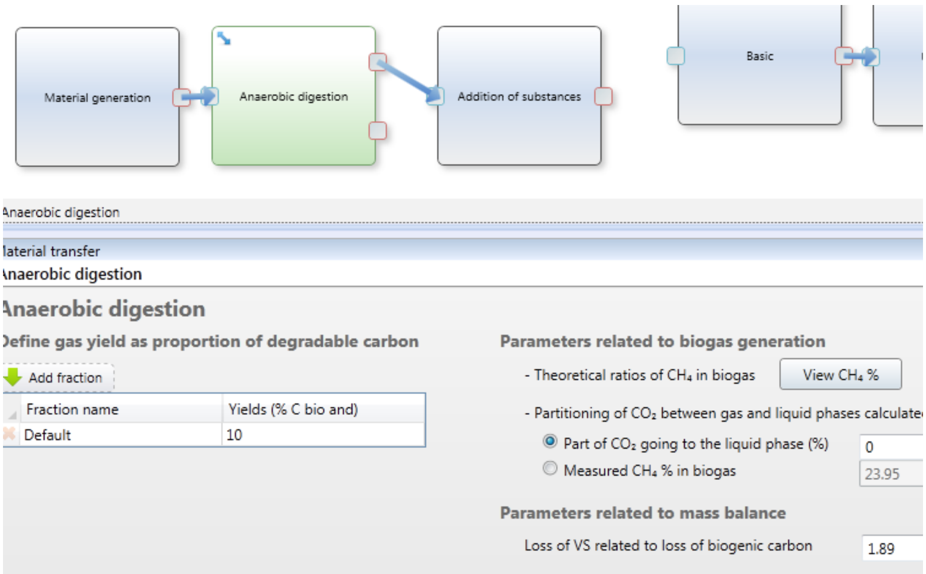
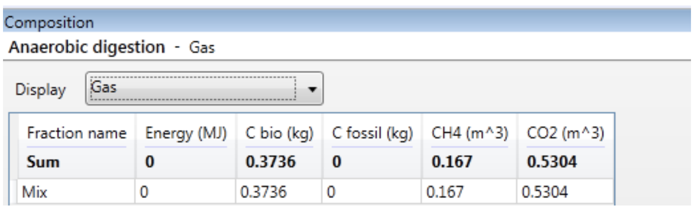


Figure S17: Material transfer of “Anaerobic digestion” process needed in the case of “gas” selection

As explained in subsection 16, the output of this AD process is as shown in Figure S18.


Composition

Anaerobic digestion - Gas

Display: Gas

Fraction name	Energy (MJ)	C bio (kg)	C fossil (kg)	CH4 (m^3)	CO2 (m^3)
Sum	**0**	**0.3736**	**0**	**0.167**	**0.5304**
Mix	0	0.3736	0	0.167	0.5304

Figure S18: Material composition of the output of the AD process (input of “addition of substance”)

So when we 0.02 g/m3 of biogas, the amount of Hg in the fraction mix is:
0.02 g *(0.167 m3+0.5304 m3)/10^3 g =1.395E-5 kg.

➢ **If we select “liquid”:**

The output is the same as the input except for Hg, which is:

- for vegetable food waste: 9.66E-8 kg + 0.02 mg /10^6 g *16.17 kg= 0.966E-7 kg + 3.234E-7 kg = 4.2E-7 kg.

- for office paper: 2.925E-7 kg + 0.0 2mg/10^6 g *0.7875 l= 2.925 E-7 kg+ 0.1575 E-7 kg = 3.0825 E-7 kg.

➢ **If we select “energy”:**

The output is the same as the input except for Hg, which is:

- for vegetable food waste: 9.66E-8 kg + 0.02 g /10^3 g *88.389 MJ = 0.966 E-7 kg + 1.77 E-3 kg = 1.77E-3 kg.

- for office paper: 2.925E-7 kg + 0.02 g / 10^3 g *103 MJ= 2.925 E-7 kg + 2.06E-3 kg = 2.06E-3 kg.

1.12 Emissions to the environment

No output.

1.13 Landfill gas generation

The user needs to specify in the “Material transfer” window of the anaerobic digestion process:

- **k rates** (in yr^{-1}) for each material fraction. They are the speed of decay of the C bio and.
- A factor that the user can change (named **number_of_years** in the rest of the text. The default value is 100.
- A factor that the user can change (named **vs_cbio** in the rest of the text). The default value is 1.89.

Principle is that we degrade **C bio and** with a first order decay. In consequence **C bio** is degraded. **CO2** and **CH4** are produced as a function of **C bio and** using the **CH4_in_biogas** property. Finally the gas produced has a lot of fractions named “year 1”, “year 2”, “year 3” etc, and C bio, CH4 and CO2 are calculated for each year and put in the corresponding fractions of the gas output.

➢ **Calculation of CH4_in_biogas property**

This is exactly the same calculation as in the anaerobic digestion module.

In the calculations of the outputs, we need to calculate for each material fraction a new material property called ch4_biogas, which is in percentage the part of C bio that is transformed into CH4 (the rest being transformed into CO2). This is calculated based on 4 other material properties named “C bio and”, “H”, O” and “N” with this formula:

Ch4_biogas = $\frac{1}{2}+\frac{168*H-21*O-36*N}{112*Cbioand}$ (the value obtained is between 0 and 1)

➢ **Calculations of the gas output**

The gas output has the number of fractions defined by the user by “number_of_years”. Each fraction is named “Year 1”, “Year 2”, etc. For year n (1 ≤ n ≤ number_of_years] these are the properties [NB: C_bio_and, k and ch4_biogas are specific for each fraction] :

- C bio [kg] is: Sum_for_all_material_fractions_of [C_bio_and * exp(- k *(n-1)) *(1-exp(- k))]
- CH4 [m3] is: Sum_for_all_material_fractions_of [C_bio_and * exp(- k *(n-1)) *(1-exp(- k)) * CH4_biogas] *22.4/12

- CO2 [m3] is: Sum_for_all_material_fractions_of [C_bio_and * exp(- k *(n-1)) *(1-exp(- k)) *(1-CH4_biogas)] *22.4/12
- All other properties are zero, including water, VS and ash.

➢ **<u>Calculation of the Residues output</u>**

The residues output has the same number of material fractions as the input. It is basically defined as equal to the input minus the carbon going to gas. For each material fraction, here are the properties [NB: k is specific to the fraction!]:

- C bio [kg] is: input.c_bio - input.c_bio_and * (1-exp(- number_of_years * k))
- C bio and is: input.c_bio_and *exp(- number_or_years*k)
- VS is: input.vs – vs_cbio *input.c_bio_and * (1-exp(- number_or_years*k))
- LHV dry [MJ]: input.lhvdry /input.vs *(input.vs – vs_cbio *input.c_bio_and * exp(- number_or_years*k))
- All other properties are equal to the input.

➢ **<u>Example:</u>**

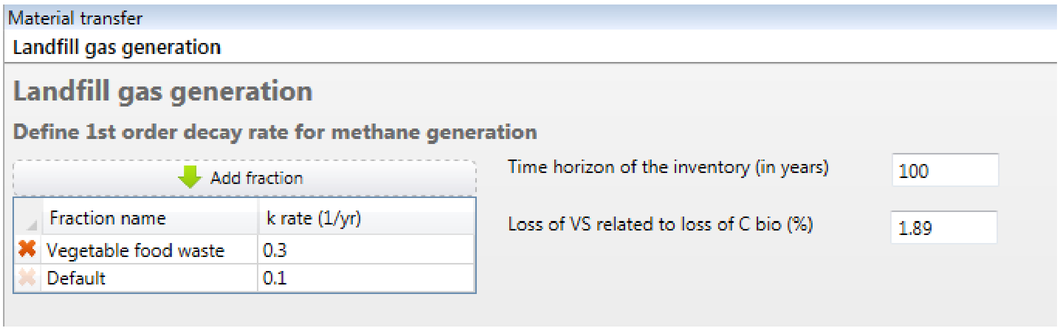


Figure S19: Material transfer of the "Landfill gas generation" process

Gas output, at year n:

- C bio [kg] is: 2.043 * exp(- 0.3 *(n-1)) *(1-exp(- 0.3)) + 1.693 * exp(- 0.1 *(n-1)) *(1-exp(- 0.1)) so for n=1, 0.6906, and for n=2, 0.5380, and sum=3.736 kg.
- CH4 [m3] is: (2.043 * exp(- 0.3 *(n-1)) *(1-exp(- 0.3)) *0.5445 + 1.693 * exp(- 0.1 *(n-1)) *(1-exp(- 0.1)) *0.5285)*22.4/12 so for n=1: 0.6971 m^3 and for n=2: 0.5425 m^3, and sum=3.746
- CO2 [m3] is: (2.043 * exp(- 0.3 *(n-1)) *(1-exp(- 0.3)) *(1-0.5445) + 1.693 * exp(- 0.1 *(n-1)) *(1-exp(- 0.1)) *(1-0.5285))*22.4/12 so for n=1: 0.5920 m^3 and for n=2: 0.4618 m^3 and sum=3.227
- All other properties are zero, including water, VS and ash.

Composition
Landfill gas generation - Gas

Display: Gas

Fraction name	Energy (MJ)	C bio (kg)	C fossil (kg)	CH4 (m^3)	CO2 (m^3)
Sum	**0**	**3.736**	**0**	**3.746**	**3.227**
Year 1	0	0.6906	0	0.6971	0.592
Year 2	0	0.538	0	0.5425	0.4618
Year 3	0	0.4225	0	0.4255	0.3632
Year 4	0	0.3346	0	0.3365	0.2881
Year 5	0	0.2675	0	0.2686	0.2306
Year 6	0	0.2159	0	0.2165	0.1865
Year 7	0	0.1759	0	0.1762	0.1522
Year 8	0	0.1448	0	0.1448	0.1255
Year 9	0	0.1204	0	0.1202	0.1045
Year 10	0	0.1011	0	0.1008	0.0879
Year 11	0	0.08562	0	0.08526	0.07457
Year 12	0	0.07315	0	0.07275	0.0638
Year 13	0	0.06299	0	0.06257	0.05501
Year 14	0	0.05462	0	0.0542	0.04775
Year 15	0	0.04766	0	0.04726	0.04171

Figure S20: Composition of the gas output from “Landfill gas generation” process

Residues output:

- C bio (vfw) =2.294 + 2.043 * (exp(- 100 * 0.3) -1) =0.251 kg
  (ofp) = 3.065 + 1.693 * (exp(- 100 * 0.1) -1) =1.372 kg
- C bio and (vfw) = 2.043 * exp(- 100 * 0.3)) =1.91E-13 kg
  (ofp) = 1.693 * exp(- 100 * 0.1)=7.68E-5 kg
- VS (vfw)= 4.579 – 1.89 *2.043 * (1-exp(- 100*0.3)) =0.718 kg
  (ofp) = 6.516 -1.89*1.693*(1-exp(-100*0.1)) = 3.316 kg
- LHV dry (vfw) = 88.39 /4.579 *(4.579 – 1. 89 *2.043 * (1-exp(- 100*0.3)))=13.85 MJ
  (ofp) = 103/6.156*(6.516 -1.89*1.693*(1-exp(-100*0.1))) =55.49 MJ
- All other properties are equal to the input.

Landfill gas generation - Residues

Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)
Sum	**22.94**	**5.986**	**16.96**	**4.034**	**1.952**	**66.26**	**1.623**	**7.685E-05**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**
Vegetable food waste	17.14	0.9686	16.17	0.7174	0.2512	13.85	0.2512	1.912E-13	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134
Office paper	5.805	5.018	0.7875	3.317	1.701	52.41	1.372	7.685E-05	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696

Figure S21: Composition of the residues output from “Landfill gas generation” process

1.14 Mass transfer over years

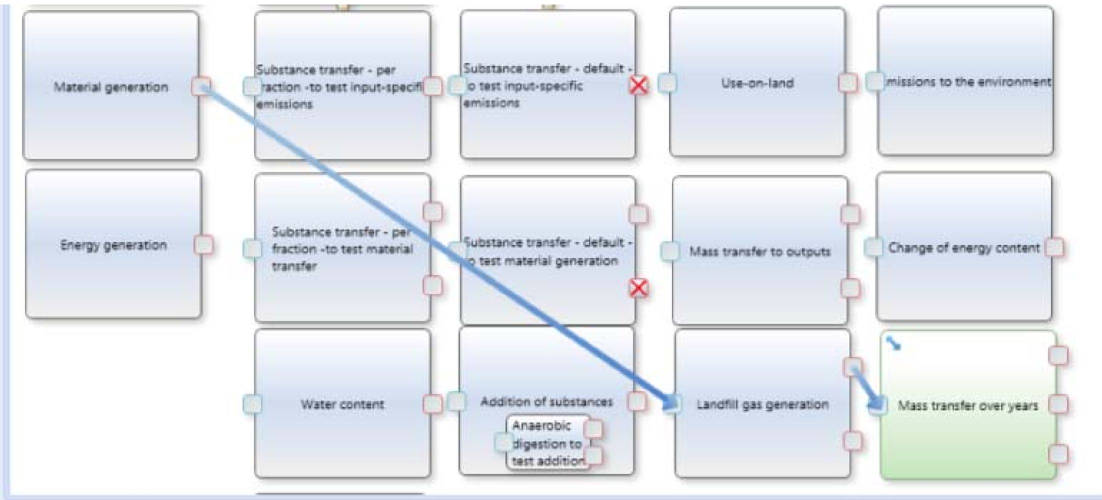
The user specifies for different time periods the routing to different outputs. Each output has as many year fractions as the input.

For each output O, for each year Y,

- Find the period P where Y is located
- all material properties are calculated as: Input.fraction.year.materialProperty *TC(P, O)/100

where TC is the transfer coefficient specified by the user in the table, for the period P and the output O.

In this example we connect this process to a landfill gas generation (Figure S22).



Material transfer

Mass transfer over years

Mass transfer over years

Time period duration (years)

Time period duratic	Half collected	Collected	Not collected
3	10	50	40
7	20	80	0
90	0	0	100

Add output column

Figure S22: Material transfer of the "Mass transfer over years" process

The input from the landfill gas generation was:

Composition

Landfill gas generation - Gas

Display: Gas

Fraction name	Energy (MJ)	C bio (kg)	C fossil (kg)	CH4 (m^3)	CO2 (m^3)
Sum	**0**	**3.736**	**0**	**3.746**	**3.227**
Year 1	0	0.6906	0	0.6971	0.592
Year 2	0	0.538	0	0.5425	0.4618
Year 3	0	0.4225	0	0.4255	0.3632
Year 4	0	0.3346	0	0.3365	0.2881
Year 5	0	0.2675	0	0.2686	0.2306
Year 6	0	0.2159	0	0.2165	0.1865
Year 7	0	0.1759	0	0.1762	0.1522
Year 8	0	0.1448	0	0.1448	0.1255
Year 9	0	0.1204	0	0.1202	0.1045
Year 10	0	0.1011	0	0.1008	0.0879
Year 11	0	0.08562	0	0.08526	0.07457
Year 12	0	0.07315	0	0.07275	0.0638
Year 13	0	0.06299	0	0.06257	0.05501
Year 14	0	0.05462	0	0.0542	0.04775
Year 15	0	0.04766	0	0.04726	0.04171
Year 16	0	0.04182	0	0.04144	0.03664
Year 17	0	0.03688	0	0.03651	0.03233
Year 18	0	0.03266	0	0.03231	0.02865
Year 19	0	0.02902	0	0.0287	0.02547
Year 20	0	0.02586	0	0.02557	0.02271
Year 21	0	0.02311	0	0.02284	0.0203

Figure S23: Material composition of the input to the "Mass transfer over years" process

So the calculations for CH4 are:

- For "Half collected" output,
  - Year 1 (period=1): 0.6971 * 10/100 =0.06971
  - Year 2 (period=1): 0.5425 *10/100 =0.05425

- Year 3 (period=1): 0.4255 *10/100 =0.04255
- Year 4 (period=2): 0.3365 *20/100 =0.0673
- …
- Year 10 (period=2): 0.1008 *20/100 =0.02016
- Year 11 (period=3): 0.08526 *0/100 =0
- …

- For "Collected" output,
  - Year 1 (period=1): 0.6971 * 50/100 =0.3485
  - Year 2 (period=1): 0.5425 *50/100 =0.2712
  - Year 3 (period=1): 0.4255 *50/100 =0.2127
  - Year 4 (period=2): 0.3365 *80/100 =0.2692
  - …
  - Year 10 (period=2): 0.1008 *80/100 =0.0806
  - Year 11 (period=3): 0.08526 *0/100 =0
  - …
- For "Not collected" output,
  - Year 1 (period=1): 0.6971 * 40/100 =0.2788
  - Year 2 (period=1): 0.5425 *40/100 =0.217
  - Year 3 (period=1): 0.4255 *40/100 =0.1702
  - Year 4 (period=2): 0.3365 *0/100 =0
  - …
  - Year 10 (period=2): 0.1008 *0/100 =0
  - Year 11 (period=3): 0.08526 *100/100 =0.08526
  - …

Concerning C bio, the C bio in year 8 of output "Half collected" is: 0.02896.

1.15 Leachate generation

There are always two outputs: leachate and residues.

Leachate has year fractions. The number of year fractions is determined by the user in the field "Time horizon of the inventory (years)". For each year Y:

- The leachate has water (kg) determined thanks to the left table. We need first to find the time period P containing the year Y:

  leachate.year.water = input.totalWetWeight *netInflitration(P) /(density *height *10^3)

  where density is the user-defined value given in "Bulk density" field
  and height is the user-defined value given in the "Height of layer" field

- Substances (kg) determined thanks to the right table: for each substance determined in the table on the right, we need to find the time period P' that contains the year Y and then the amount of substance in that year Y is:

  leachate.year.substance = leachate.year.water *concentrate(substance, P')*10^-6
  or if easier:
  leachate.year.substance = input.totalWetWeight *netInflitration(P) /(density *height *10^3) *concentrate(substance, P')*10^-6

where density is the user-defined value given in “Bulk density” field
and height is the user-defined value given in the “Height of layer” field

Residues is equal to the input minus the substances that go in the leachate. For all substances of input, for each material fraction, the amount in “residues” is:

If **input.substance(of_all_fractions =0, then it is zero, else:**

Input.fraction.substance – sum_for_all_years [leachate.year.water *concentrate(substance, P’)*10^-6] *input.fraction.substance/input.substance(of_all_fractions))

When connecting the process described in Figure

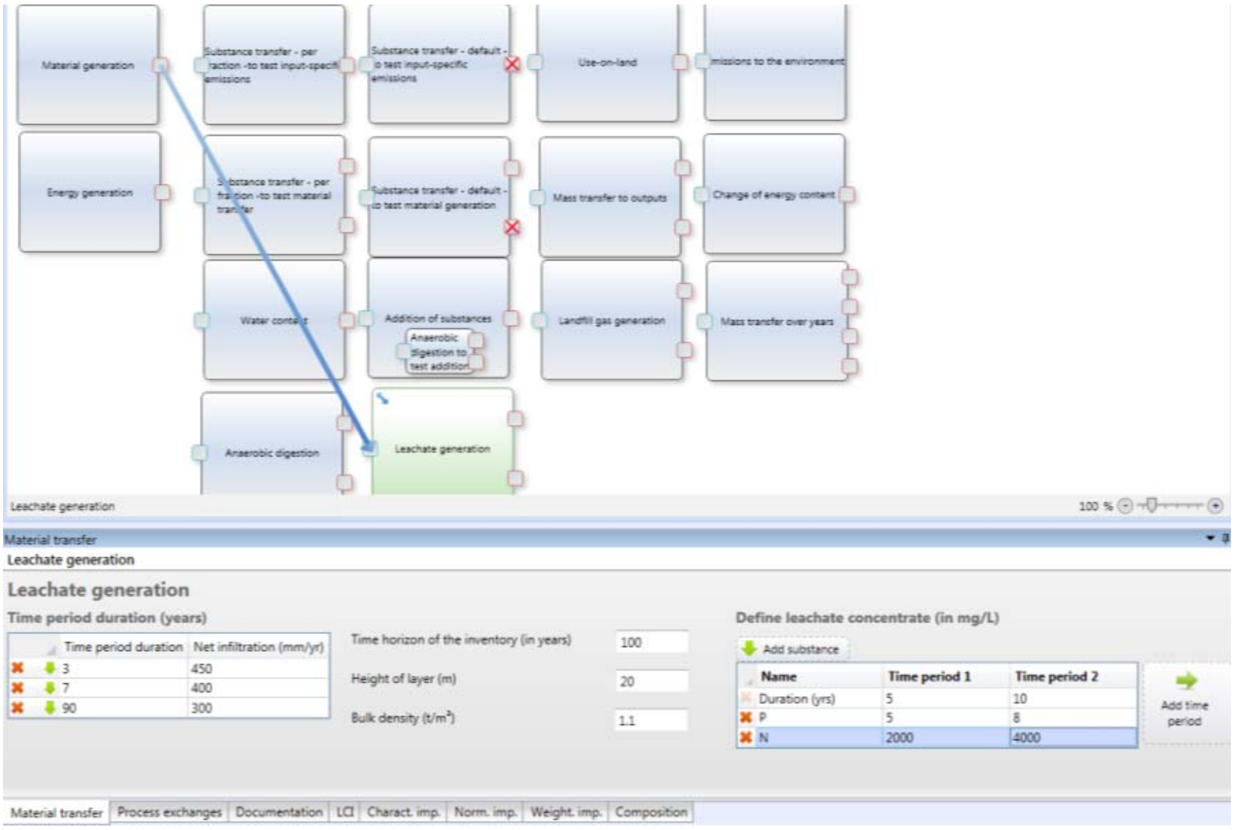


Figure S24: Material transfer of the “Leachate generation” process

So the calculations for water and N are:

- For “Leachate” output, the water is:
    - Year 1 (period=1): 30 *450 /(1.1 *20 *10^6) =0.614 kg
    - Year 2 (period=1): 30 *450 /(1.1 *20 *10^6) =0.614 kg
    - Year 3 (period=1): 30 *450 /(1.1 *20 *10^6) =0.614 kg
    - Year 4 (period=2): 30 *400 /(1.1 *20 *10^6) =0.545 kg
    - …
    - Year 10 (period=2): 30 *400 /(1.1 *20 *10^6) =0.545 kg
    - Year 11 (period=3): 30 *300 /(1.1 *20 *10^6) =0.409 kg
    - …
- For “leachate” output, N is:
    - Year 1 (period=1, P’=1): 30 *450 /(1.1 *20 *10^3) *2000E-6 =1.227E-3 kg

- Year 2 (period=1, P’=1): 30 *450 /(1.1 *20 *10^3) *2000E-6 =1.227E-3 kg
- Year 3 (period=1, P’=1): 30 *450 /(1.1 *20 *10^3) *2000E-6 =1.227E-3 kg
- Year 4 (period=2, P’=1): 30 *400 /(1.1 *20 *10^3) *2000E-6 =1.091E-3 kg
- Year 5 (period=2, P’=1): 30 *400 /(1.1 *20 *10^3) *2000E-6 =1.091E-3 kg
- Year 6 (period=2, P’=2): 30 *400 /(1.1 *20 *10^3) *4000E-6 =2.182E-3 kg
- …
- Year 10 (period=2, P’=2): 30 *400 /(1.1 *20 *10^3) *4000E-6 =2.182E-3 kg
- Year 11 (period=3, P’=2): 30 *300 /(1.1 *20 *10^3) *4000E-6 =1.636E-3 kg
- …
- Year 16 (period=3, P’=3): 30 *300 /(1.1 *20 *10^3) *0 =0 kg

- For “Residues” output, all properties are the same as the input except from N and P, lets’ check for N:
  - Vegetable food waste: 0.09175 – sum_for_all_years[leachate.year.water *concentrate(N, P’)*10^-6] *0.09175/0.09996)
    = 0.09175 – [3*1.227E-3 +2*1.091E-3 +5*2.182E-3 +5*1.636E-3] *0.09175/0.09996
    =0.0688 kg
  - Office paper: 0.008217 – sum_for_all_years[leachate.year.water *concentrate(N, P’)*10^-6] *0.008217/0.09996)
    = 0.008217 – [3*1.227E-3 +2*1.091E-3 +5*2.182E-3 +5*1.636E-3] *0.008217/0.09996
    =0.006166 kg

Composition

Leachate generation - Leachate

Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)
Sum	**42.48**	**0**	**42.48**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0.02496**	**0**
Year 1	0.6137	0	0.6137	0	0	0	0	0	0	0	0	0	0	0	0.001227	0
Year 2	0.6137	0	0.6137	0	0	0	0	0	0	0	0	0	0	0	0.001227	0
Year 3	0.6137	0	0.6137	0	0	0	0	0	0	0	0	0	0	0	0.001227	0
Year 4	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.001091	0
Year 5	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.001091	0
Year 6	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.002182	0
Year 7	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.002182	0
Year 8	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.002182	0
Year 9	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.002182	0
Year 10	0.5455	0	0.5455	0	0	0	0	0	0	0	0	0	0	0	0.002182	0
Year 11	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0.001636	0
Year 12	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0.001636	0
Year 13	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0.001636	0
Year 14	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0.001636	0
Year 15	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0.001636	0
Year 16	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0	0
Year 17	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0	0
Year 18	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0	0
Year 19	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0	0
Year 20	0.4091	0	0.4091	0	0	0	0	0	0	0	0	0	0	0	0	0

Composition

Leachate generation - Residues

Display: Default

Fraction name	bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)	S (kg)	Hg (kg)
Sum	**.736**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**	**0.07503**	**0.02143**	**4.923**	**0.01142**	**0.01417**	**3.891E-07**
Vegetable food waste	043	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134	0.06886	0.01507	1.908	0.01111	0.008887	9.66E-08
Office paper	693	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696	0.006166	0.00636	3.016	0.0003124	0.005284	2.925E-07

Figure S25: Composition of the two outputs of the “leachate generation” process

1.16 Anaerobic digestion

This process has two outputs called "gas" and "digestate". The user needs to specify in the "Material transfer" window of the anaerobic digestion process:

- **Yields** (in %) for each material fraction. They describe how much of the "C bio and" is actually degraded in the digester. Like in the other tables, there is always a "default" fraction, and the user can add and delete lines (i.e. fractions).
- A factor called "Loss of VS related to loss of C bio" (named **vs_cbio** in the rest of the text). Default value: 1.89.
- A factor called "Part of CO2 going to the liquid phase (%)" (named **co2_liq** in the rest of this text). The default value is zero.
- A list of **pollutants** and their transfer coefficients (TC) from the input to the gas and digestate outputs, given by the user in **kg/Nm3 biogas**. The user selects the material property and writes a transfer coefficient in the column "Gas" for the default fraction line (and possibly to specific fractions), the value in the column "digestate" is automatically calculated as "100-TCgas". By default everything goes to digestate. NB: VS, Cbio, Cbioand and energy cannot be changed in this table because they are calculated based on the other parameters.

➢ **Calculation of CH4 for each material fractions (shown when clicking on button "View CH4%")**

In the calculations of the outputs, we need to calculate for each material fraction a material property called **ch4_biogas**, which is in percentage the part of C bio that is transformed into CH4 (the rest being transformed into CO2). This is calculated based on 4 other material properties named "C bio and", "H", O" and "N" with this formula:

Ch4_biogas = $\frac{1}{2}+\frac{168*H-21*O-36*N}{112*Cbioand}$ (the value obtained is between 0 and 1)

➢ **Calculation of "Part of CO2 liquid" and "Measured CH4" depending on radio buttons**

- When the first radiobutton is selected: the user edits co2_liq and measuredCH4% is calculated

MeasuredCH4% is CH4 divided by biogas:

100* Sum_for_all_material_fractions_of (yield/100 * C_bio_and * ch4_biogas/100) /

[Sum_for_all_material_fractions_of (yield/100 * C_bio_and * ch4_biogas/100) + Sum_for_all_material_fractions_of (yield/100 * C_bio_and * (1-ch4_biogas/100)) *(1-co2_liq/100)]

- When the second radiobutton is selected: the user edits measuredCH4% and co2liq is calculated

Co2liq is calculated like this:

100 – (100-measured_ch4%) / measured_ch4% * Sum_for_all_material_fractions_of (yield/100 * C_bio_and * ch4_biogas/100) / Sum_for_all_material_fractions_of (yield/100 * C_bio_and * (1-ch4_biogas/100))

➢ **Calculation of the GAS output**

The gas output has one fraction called "Mix" with these properties:

- C bio [kg] is: Sum_for_all_material_fractions_of (yield/100 * C_bio_and *(1– co2_liq/100*(1-ch4_biogas/100)))

- CH4 [m3] is: Sum_for_all_material_fractions_of (yield/100 * C_bio_and * ch4_biogas/100)*22.4/12
- CO2 [m3] is: Sum_for_all_material_fractions_of : (yield/100 * C_bio_and * (1-ch4_biogas/100)) *(1-co2_liq/100) *22.4/12
- Pollutants [kg]: Sum_for_all_material_fractions_of (pollutant_kg(fraction)*TC_of_pollutants_to_gas/100)
- All other properties are zero, including water, VS, ash, Energy, C bio and.

➢ **<u>Calculation of the DIGESTATE output</u>**

The digestate output has the same number of material fractions as the input, and their names. It is defined as equal to the input minus what goes to the gas (I write "input." to designate properties of the input material). For each material fraction, here are the properties:

- C bio [kg] is: input.c_bio – input.C_bio_and *yield/100 *(1- co2_liq/100*(1-ch4_biogas/100)
- C bio and is: input.c_bio_and*(1 -yield/100)
- VS is: input.vs – vs_cbio *C_bio_and *yield/100
- LHV dry [MJ] is: input.lhvdry /input.vs *(input.vs – vs_cbio *C_bio_and *yield/100)
- For pollutants with defined transfer coefficients: pollutant [kg] = input.pollutant*TC_to_digestate/100
- All other properties are equal to the input, including water and ash.

➢ **<u>Example:</u>**

We use the example of 30 kg of 70 % vegetable food waste and 30 % office paper (Table S1). The theoretical CH4 ratios are: 54.45 % for vegetable food waste and 52.85 % for office paper.

a. <u>With radio button on "Part of CO2…"</u>

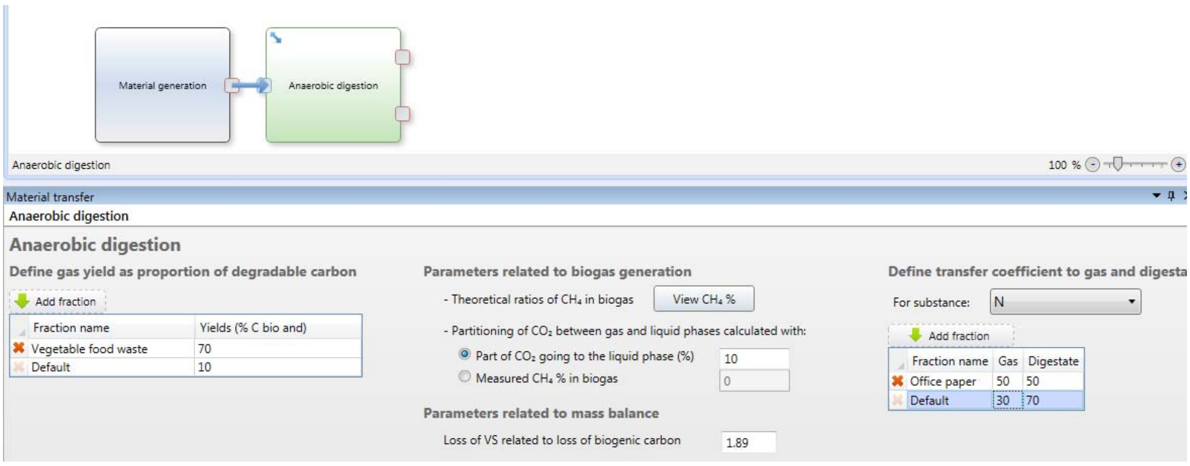


Figure S26: Material transfer of the "anaerobic digestion" process

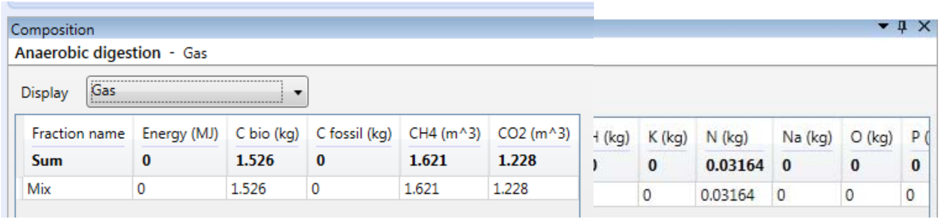
The value "Measured CH4% in biogas" is:

100* (70/100 * 2.043 * 54.45/100 + 10/100 * 1.693 * 52.85/100) / [(70/100 * 2.043 * 54.45/100 + 10/100 * 1.693 * 52.85/100) + (70/100 * 2.043 * (1-54.45/100) + 10/100 * 1.693 * (1-52.85/100)) *(1-10/100)] = 56.88

The gas output is:

- C bio [kg] = 70/100 * 2.043 * (1-10/100*(1-54.45/100)) + 10/100 * 1.693 * (1-10/100*(1-52.85/100)) =1.526 kg

- CH4 [m3]= (70/100 * 2.043 * 54.45/100 + 10/100 * 1.693 * 52.85/100)*22.4/12 = 1.621 m^3
- CO2 [m3] =(70/100 * 2.043 * (1-54.45/100) + 10/100 * 1.693 * (1-52.85/100))*(1-10/100)*22.4/12 =1.228 m^3
- N [kg]: 0.09177*30/100 + 0.008217*50/100 = 0.03164 kg



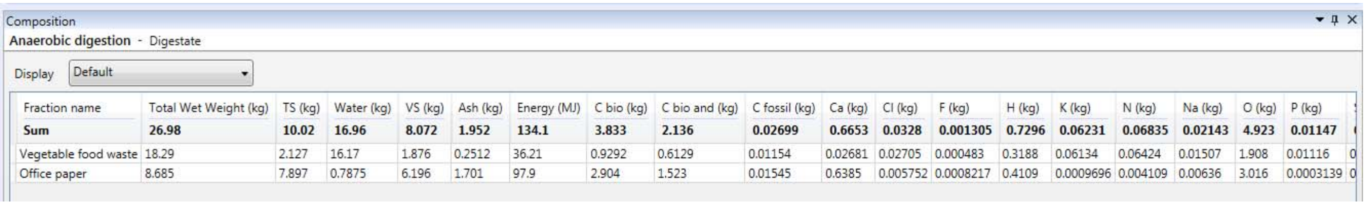
Composition
Anaerobic digestion - Gas
Display: Gas

Fraction name	Energy (MJ)	C bio (kg)	C fossil (kg)	CH4 (m^3)	CO2 (m^3)	K (kg)	N (kg)	Na (kg)	O (kg)
Sum	**0**	**1.526**	**0**	**1.621**	**1.228**	**0**	**0.03164**	**0**	**0**
Mix	0	1.526	0	1.621	1.228	0	0.03164	0	0

Figure S27: Composition of the gas output

The digestate output is:

- C bio (vfw)= 2.294 - 2.043 *70/100 *(1-10/100*(1-54.45/100))= 0.929 kg
  (ofp)= 3.065 - 1.693*10/100 *(1-10/100*(1-52.85/100)) =2.904 kg
- C bio and (vfw) = 2.043 *(1-70/100) = 0.613 kg
  (ofp)= 1.693*(1-10/100) = 1.524 kg
- VS (vfw) = 4.579 - 1.89*2.043 *70/100 = 1.876 kg
  (ofp) = 6.516 -1.89*1.693*10/100 = 6.196 kg
- LHV dry (vfw) = 88.389/4.579*(4.579 - 1.89*2.043 *70/100) = 36.21 MJ
  (ofp) = 103/6.516*(6.516 -1.89*1.693*10/100) = 97.94 MJ
- N (vfw) =0.09177* 70/100 =0.06424 kg
  (ofp) = 0.008217*50/100 = 0.004109 kg
- All other properties are equal to the input



Composition
Anaerobic digestion - Digestate
Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (kg)
Sum	**26.98**	**10.02**	**16.96**	**8.072**	**1.952**	**134.1**	**3.833**	**2.136**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**	**0.06835**	**0.02143**	**4.923**	**0.01147**
Vegetable food waste	18.29	2.127	16.17	1.876	0.2512	36.21	0.9292	0.6129	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134	0.06424	0.01507	1.908	0.01116
Office paper	8.685	7.897	0.7875	6.196	1.701	97.9	2.904	1.523	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696	0.004109	0.00636	3.016	0.0003139

Figure S28: Composition of the digestate output

b. <u>With radio button on “Part of CO2…” (only this changes)</u>

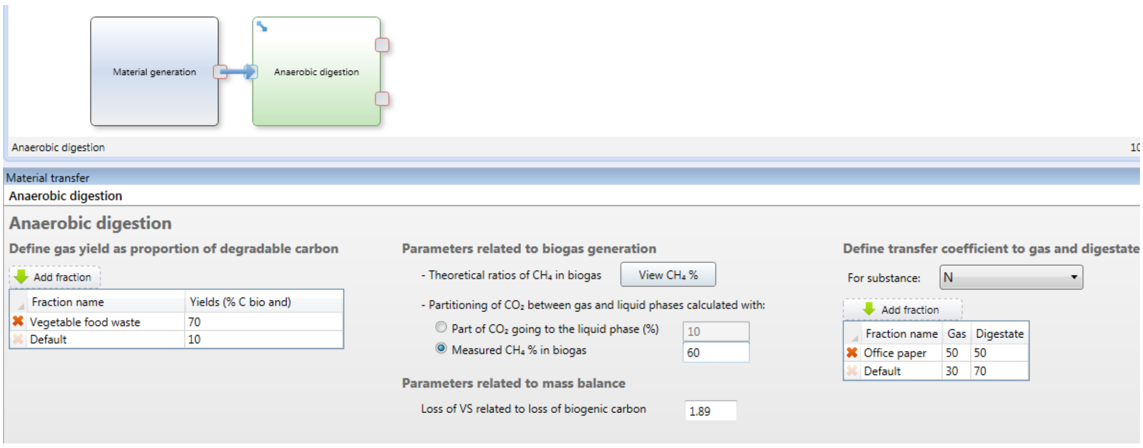


Figure S29: Material transfer of the “anaerobic digestion” process

The value “Part of CO2 going…” is:

100 – 100*(100-60)/60 * (70/100 * 2.043 * 54.45/100 + 10/100 * 1.693 * 52.85/100) / (70/100 * 2.043 * (1-54.45/100) + 10/100 * 1.693 * (1-52.85/100)) = 20.84

All the other calculations are the same as before. The gas output is:

- C bio [kg] = 70/100 * 2.043 * (1-20.84/100*(1-54.45/100)) + 10/100 * 1.693 * (1-20.84/100*(1-52.85/100)) =1.447 kg
- CH4 [m3]= (70/100 * 2.043 * 54.45/100 + 10/100 * 1.693 * 52.85/100)*22.4/12 = 1.621 m^3
- CO2 [m3] =(70/100 * 2.043 * (1-54.45/100) + 10/100 * 1.693 * (1-52.85/100))*(1-20.84/100)*22.4/12 =1.0805 m^3
- N [kg]: 0.09177*30/100 + 0.008217*50/100 = 0.03164 kg

Composition
Anaerobic digestion - Gas
Display: Gas

Fraction name	Energy (MJ)	C bio (kg)	C fossil (kg)	CH4 (m^3)	CO2 (m^3)	(kg)	K (kg)	N (kg)	Na (kg)	O (kg)	P (
Sum	**0**	**1.432**	**0**	**1.621**	**1.053**	**)**	**0**	**0.03164**	**0**	**0**	**0**
Mix	0	1.432	0	1.621	1.053		0	0.03164	0	0	0

Figure S30: Composition of the gas output

The digestate output is:

- C bio (vfw)= 2.294 - 2.043 *70/100 *(1-20.84/100*(1-54.45/100))= 0.9997 kg
  (ofp)= 3.065 - 1.693*10/100 *(1-20.84/100*(1-52.85/100)) =2.912 kg
- C bio and (vfw) = 2.043 *(1-70/100) = 0.613 kg
  (ofp)= 1.693*(1-10/100) = 1.524 kg
- VS (vfw) = 4.579 - 1.89*2.043 *70/100 = 1.876 kg
  (ofp) = 6.516 -1.89*1.693*10/100 = 6.196 kg
- LHV dry (vfw) = 88.389/4.579*(4.579 - 1.89*2.043 *70/100) = 36.21 MJ
  (ofp) = 103/6.516*(6.516 -1.89*1.693*10/100) = 97.94 MJ
- N (vfw) =0.09177* 70/100 =0.06424 kg
  (ofp) = 0.008217*50/100 = 0.004109 kg
- All other properties are equal to the input

Composition
Anaerobic digestion - Digestate
Display: Default

Fraction name	Total Wet Weight (kg)	TS (kg)	Water (kg)	VS (kg)	Ash (kg)	Energy (MJ)	C bio (kg)	C bio and (kg)	C fossil (kg)	Ca (kg)	Cl (kg)	F (kg)	H (kg)	K (kg)	N (kg)
Sum	**26.98**	**10.02**	**16.96**	**8.072**	**1.952**	**134.1**	**3.927**	**2.136**	**0.02699**	**0.6653**	**0.0328**	**0.001305**	**0.7296**	**0.06231**	**0.06835**
Vegetable food waste	18.29	2.127	16.17	1.876	0.2512	36.21	1.013	0.6129	0.01154	0.02681	0.02705	0.000483	0.3188	0.06134	0.06424
Office paper	8.685	7.897	0.7875	6.196	1.701	97.9	2.914	1.523	0.01545	0.6385	0.005752	0.0008217	0.4109	0.0009696	0.004109

Figure S31: Composition of the digestate output

Figure S32 provides explanations about the calculations happening in the anaerobic digestion process.

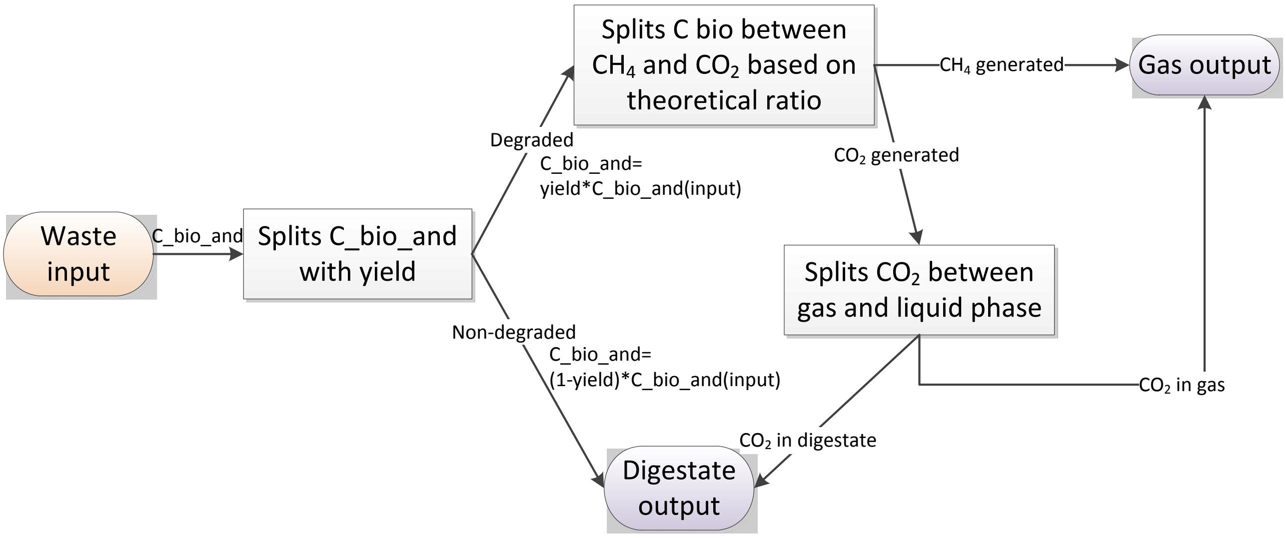


Figure S32: Calculations in the “Anaerobic digestion” process

1.17 Use-on-land

If the tickbox is ticked in “Material transfer”, the process has one output defined as the exact opposite of the input, i.e. for each material property of the input of value x, the material property of the output has a value “–x”. If the tickbox is not ticket, there is no output.

2 LCA calculations in all processes: process-specific emissions and external processes

Here we explain how the calculations are performed in material processes and external processes, concerning all data specified in the "Process exchanges" tab. Note that some material processes templates include also emissions happening in the "Material transfer" tab, these calculations are detailed in Section 3. The steps of characterization, normalization and weighting are always the same, and are thus only explained in Section 2.

The example which will be used in Section 2 is presented in Figure S33. Throughout the example we will use an impact category called "IPCC 2007, climate change, GWP 100a" which has characterisation factors of 1 for "carbon dioxide, fossil, air, unspecified" and 25 for "Methane, fossil, air, unspecified" (kg CO_2-eq/kg).

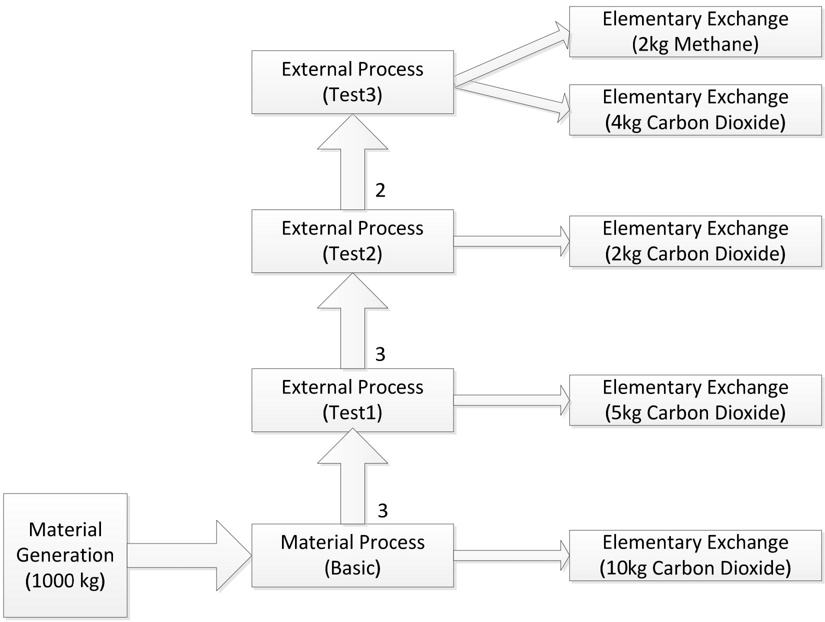


Figure S33: Example used in Section 2

2.1 An external process with only process-specific emissions: test3

The external process "test3" is presented in Figure S34. It has two process-specific emissions (we call all elementary exchanges in the "Process exchanges" tab of a process "process-specific" as they are related to the process being operated):

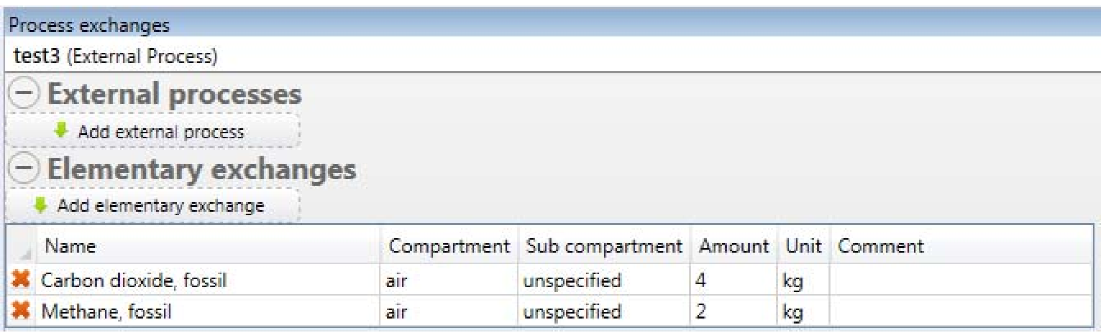
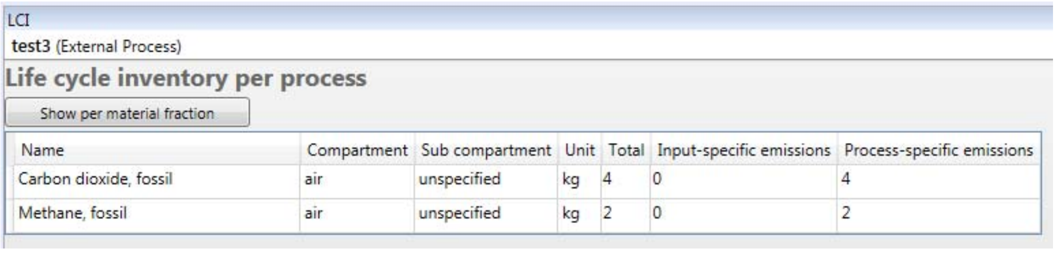


Figure S34: Process exchanges in external process test3

The LCI of an external process such as "test3" is presented in Figure S35 and calculated as:

- All elementary exchanges which are directly in the "Process exchange" tab of "test3" are called "Process-specific emissions" and are simply put directly in the LCI (see the 6th column below).
- For each external process used (in "test3" none), bring the LCI of the process (explained in Section 2.2 with "test2" process).
- The total column (5th column) shows simply the sum for all columns for the functional unit for the process.

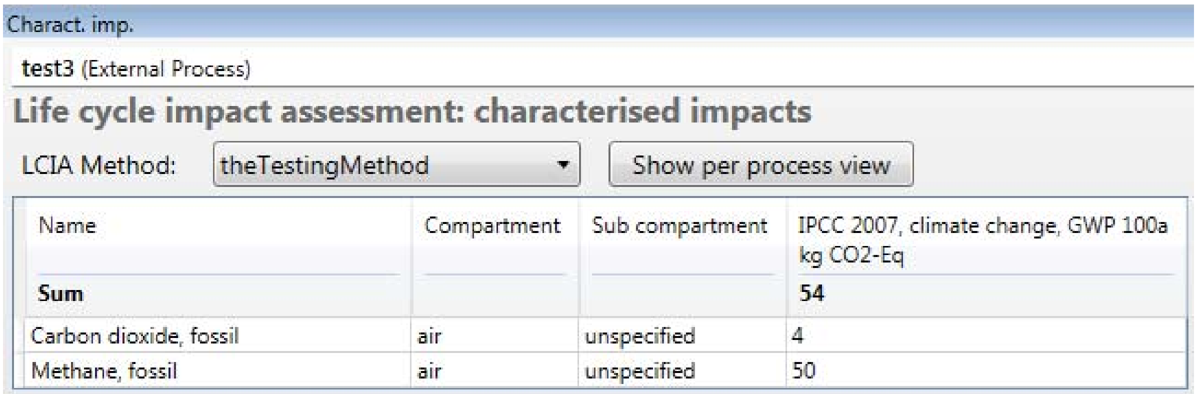

LCI
test3 (External Process)
Life cycle inventory per process
Show per material fraction

Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions
Carbon dioxide, fossil	air	unspecified	kg	4	0	4
Methane, fossil	air	unspecified	kg	2	0	2

Figure S35: LCI of external process test3

In the characterized impacts, "per substance" view, the calculation is taking the LCI line by line: for each elementary exchange of the LCI, multiply the total amount by the characterization factor of the impact category. So for "test3" characterised impacts are presented in Figure S36 and calculated as:

- Carbon dioxide: amountOfCarbonDioxideInLCI*CharacterisationFactorOfCarbonDioxide = 4*1=4
- Methane, fossil: amountOfMethaneInLCI*CharacterisationFactorOfMethane = 2*25=50


Charact. imp.
test3 (External Process)
Life cycle impact assessment: characterised impacts
LCIA Method: theTestingMethod
Show per process view

Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**54**
Carbon dioxide, fossil	air	unspecified	4
Methane, fossil	air	unspecified	50

Figure S36: Characterised impacts, per substance, of external process test3

In the characterized impacts, "per process" view, we take the LCI results column per column: for each subprocess, calculate the total impact as the sum (for all elementary exchanges) of their amount multiplied by the characterization factor.

In "test3", there is only one sub-process called "Process-specific emissions" and it is contributing to: amountOfCarbonDioxideInLci(Process specific emissions)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCI(Process specific emissions)*CharacterisationFactorOfMethane = 4*1+2*25=54

Results are shown in Figure S37. If "test3" was calling another external process, we would do the same calculation for this process (see the example in section 2.2).

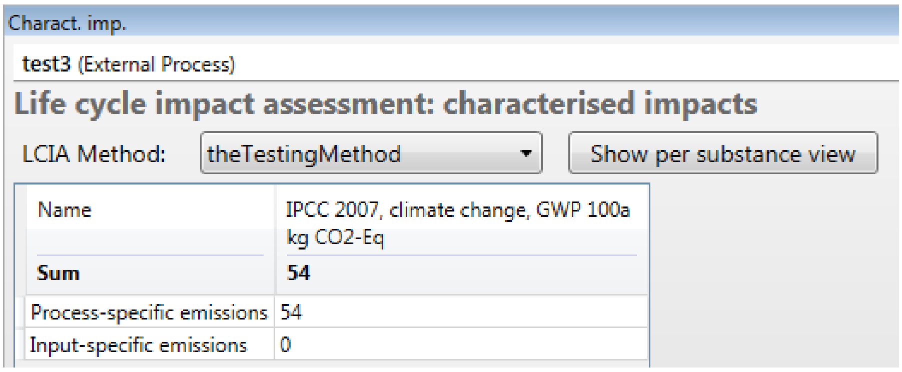


Figure S37: Characterised impacts, per process, of external process test3

2.2 An external process with process-specific emissions and one external process: test2

Figure S38 presents the external process "test2".

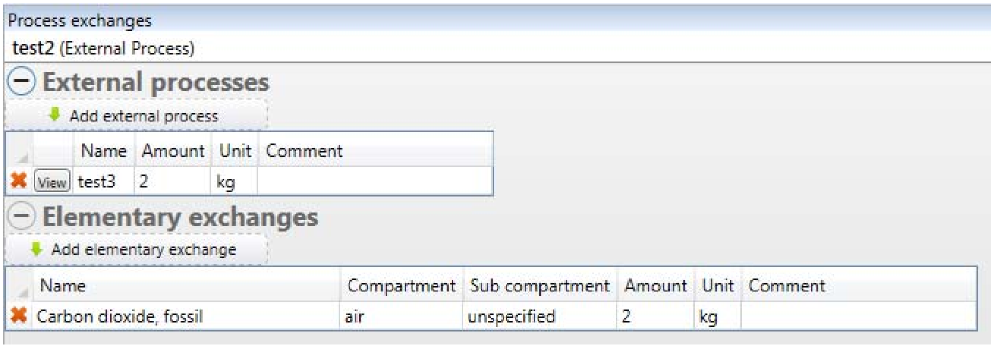


Figure S38: Process exchanges in external process test2

The LCI of "test2" has now two subprocesses: "Process specific emissions" and "test3". It is shown in Figure S39 and calculated as:

- All elementary exchanges which are directly in the "Process exchanges" tab of "test2" are called "Process-specific emissions" and are simply put directly in the LCI (see the 6th column below),
- For each external process used, you have to multiply the LCI of the process by the amount. In our example, "test2" uses 2 kg of test3 so in the column "test3" we have:
  - o Carbon dioxide: amount(test3UsedInTest2)* amountOfCarbonDioxideInLci(test3)=2*4=8.
  - o Methane: amount(test3UsedInTest2)* amountOfMethaneInLci(test3)=2*2=4.

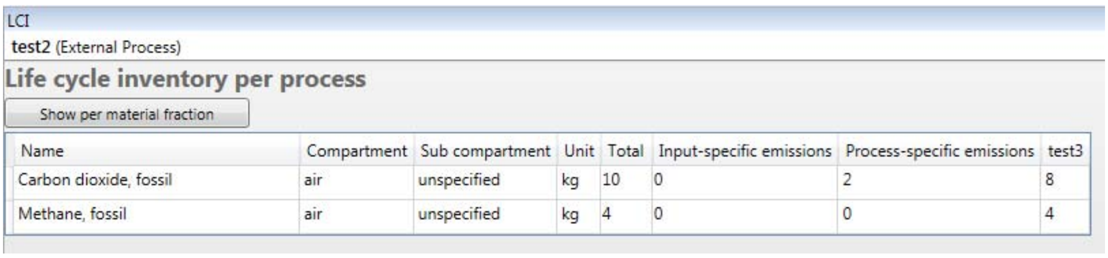
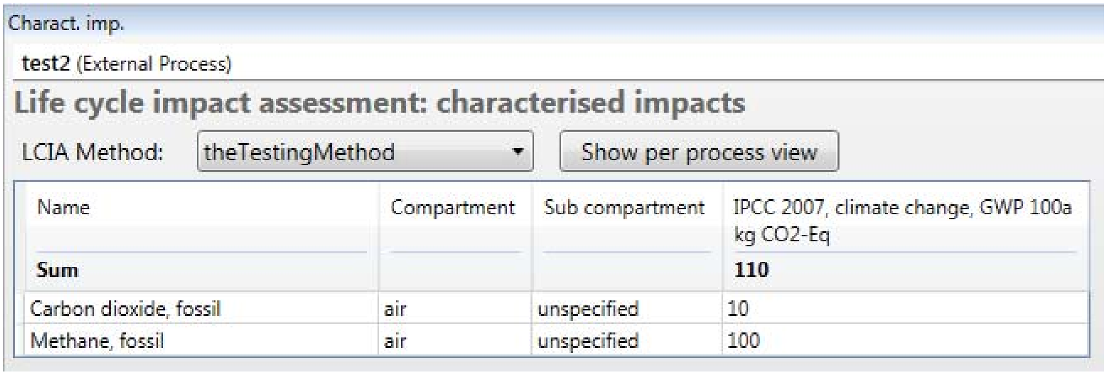


Figure S39: LCI of external process test2

In the characterized impacts per substance (Figure S40) the calculation is the following:

- Carbon dioxide: amountOfCarbonDioxideInLCI*CharacterisationFactorOfCarbonDioxide =10*1=10.
- Methane: amountOfMethaneInLCI*CharacterisationFactorOfMethane =4*25=100.


Charact. imp.

test2 (External Process)

Life cycle impact assessment: characterised impacts

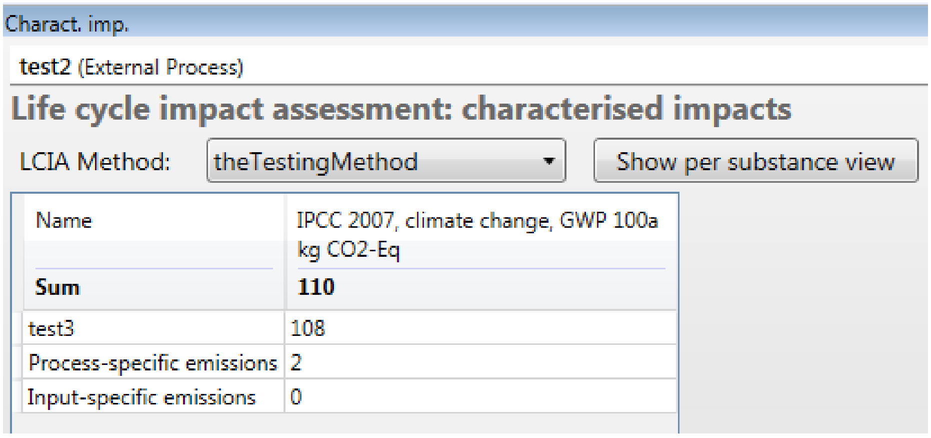
LCIA Method: theTestingMethod | Show per process view

Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**110**
Carbon dioxide, fossil	air	unspecified	10
Methane, fossil	air	unspecified	100

Figure S40: Characterised impacts, per substance, of external process test2

In the characterized impacts per process (Figure S41) the details of each subprocess "test3" and "process-specific emission" are calculated:

- For the subprocess "test3": amountOfCarbonDioxideInLCIPerProcess(Test3)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(Test3)*CharacterisationFactorOfMethane = 8*1 + 4*25=108
- For Process-specific emissions: amountOfCarbonDioxideInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfMethane = 2*1 + 0*25=2


Charact. imp.

test2 (External Process)

Life cycle impact assessment: characterised impacts

LCIA Method: theTestingMethod | Show per substance view

Name	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum	**110**
test3	108
Process-specific emissions	2
Input-specific emissions	0

Figure S41: Characterised impacts, per process, of external process test2

2.3 An external process with process-specific emissions and an external process that uses another external process: test1

Figure S42 presents "test1" an external process that uses "test2".

Figure S42: Process exchanges in external process test1

The LCI of "test1" is shown in Figure S43(again it has two sub-processes). The calculation is the same as in section 2.2:

- All elementary exchanges which are directly in the "Process exchanges" tab of "test1" are called "Process-specific emissions" and are simply put directly in the LCI (see the 6th column below),
- For each external process used, you have to multiply the LCI of the process by the amount. In our example, "test1" uses 3 kg of test2 so in the column "test2" we have:
  - o Carbon dioxide: amount(test2UsedInTest1)* amountOfCarbonDioxideInLCI(test2)=3*10=30
  - o Methane: amount(test2UsedInTest1)* amountOfMethaneInLCI(test2)=3*4=12

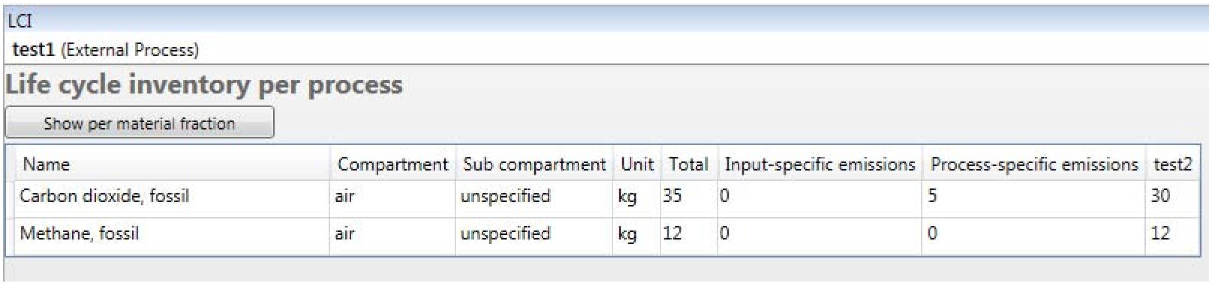


Figure S43: LCI of external process test1

In the characterized impacts per substance (Figure S44) the calculation is:

- Carbon dioxide: amountOfCarbonDioxideInLci*CharacterisationFactorOfCarbonDioxide =35*1=35
- Methane: amountOfMethaneInLci*CharacterisationFactorOfMethane =12*25=300

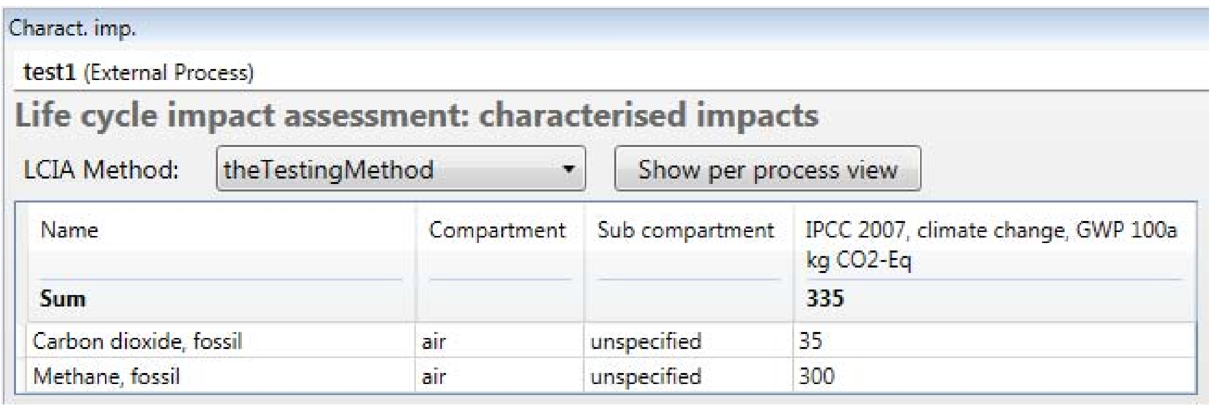


Figure S44: Characterised impacts, per substance, of external process test1

In the characterized impacts per process (Figure S45) the details of each subprocess: “test2” and “process-specific emission” are calculated:

- Test2: amountOfCarbonDioxideInLCIiPerProcessOfTest2*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcessOfTest2*CharacterisationFactorOfMethane = 30*1 + 12*25=330
- Process specific emissions: amountOfCarbonDioxideInLCIPerProcessOfProcessSpecific*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcessOfProcessSpecific*CharacterisationFactorOfMethane = 5*1 + 0*25=5

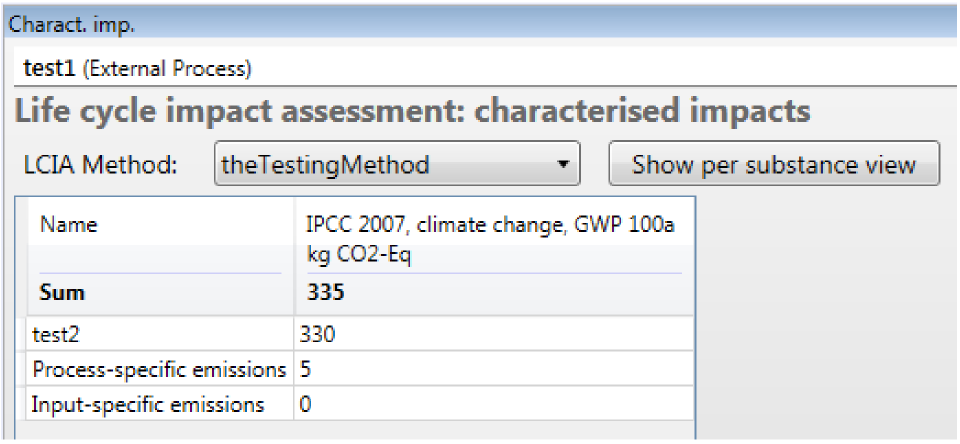


Figure S45: Characterised impacts, per process, of external process test1

2.4 A material process uses this external process

The scenario presented in Figure S46 has 1000 kg waste (100% vegetable food waste) going to a basic process that uses -3 kg of test1 per MJ energy input and emits 10 kg of carbon dioxide.

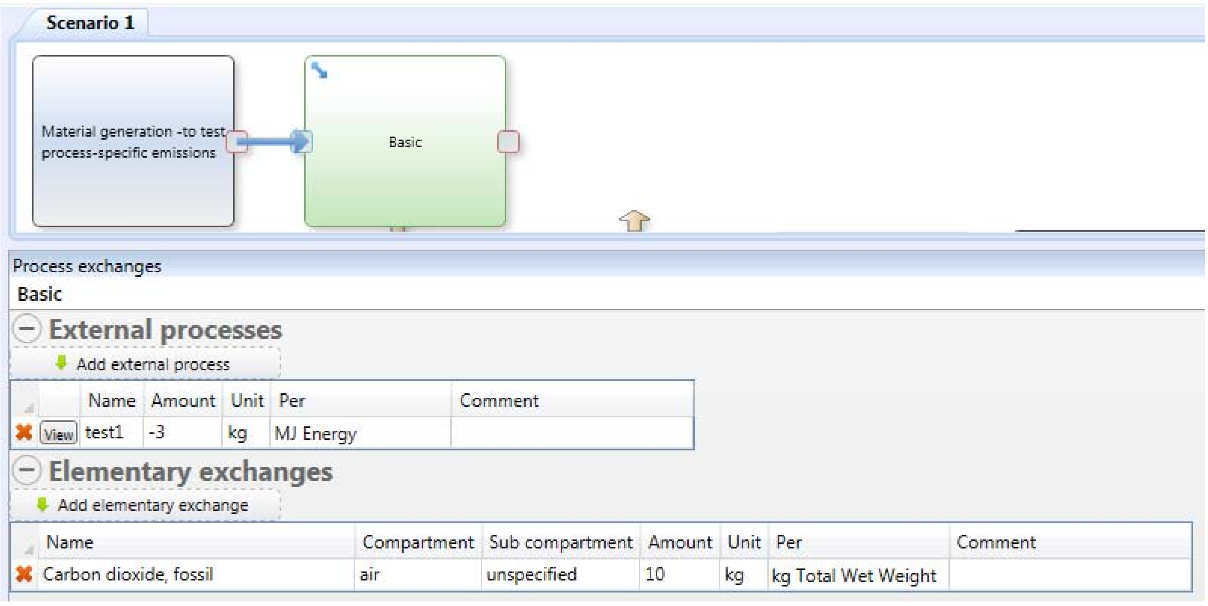


Figure S46: Process exchanges in basic process

The LCI of material processes is similar to the one of external processes (Figure S47):

- All elementary exchanges which are in the “Process exchanges” tab of “Basic” are called “Process-specific emissions”. Their amount in the LCI is:

*“Amount”_field * amount_of_the_selected_material_property_in_input_material*

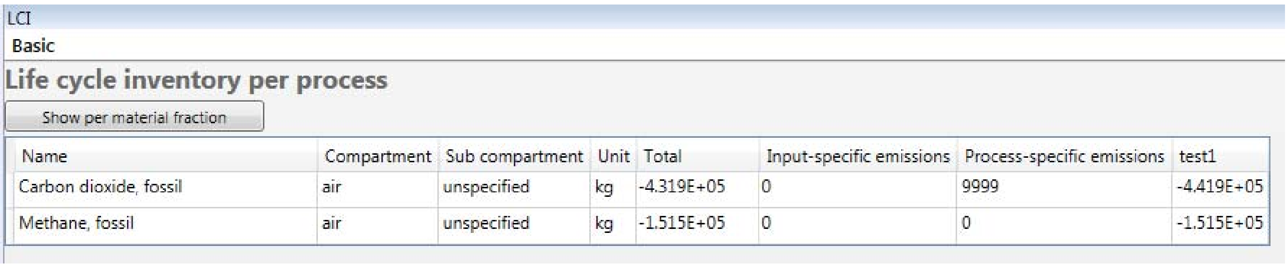
In our example, we emit 10 kg carbon dioxide per kg total wet weight (here equal to 1000) so we emit: 10*1000=1E4 kg.

- For each external process used, we get its LCI by:

  *LCI_of_the_external_process *“Amount”_field*
  **amount_of_the_selected_material_property_in_input_material*

  In our example, we use -3 kg of test1 per MJ of Energy of the input (here equal to 4209 MJ), so we calculate in the 6th column:

  - Carbon dioxide: amountOfCarbonDioxideInLCI(test1) *amount(test1UsedInBasic) *Energy(input) = 35 *(-3) *4209 = -4.419E5
  - Methane: amountOfMethaneInLCI(test1) *amount(test1UsedInBasic) * Energy(input) =12 *(-3)*4209 = -1.515E5

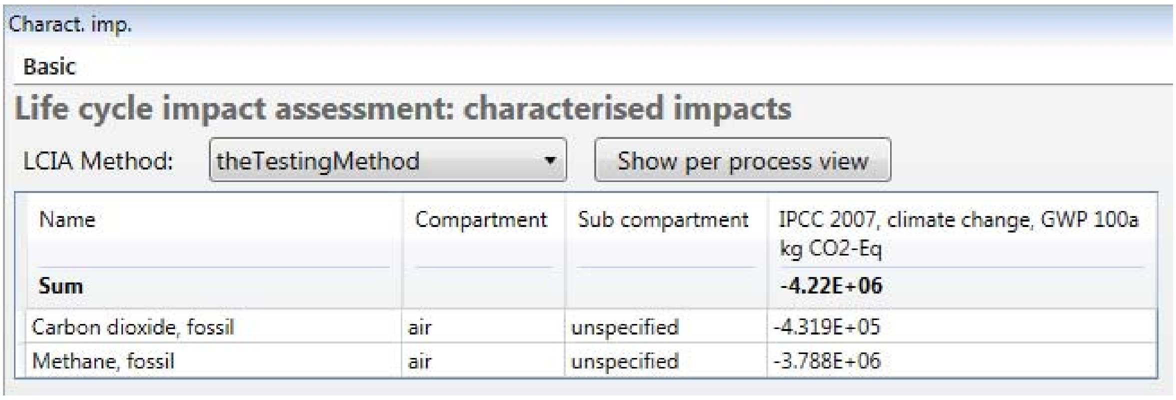


Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions	test1
Carbon dioxide, fossil	air	unspecified	kg	-4.319E+05	0	9999	-4.419E+05
Methane, fossil	air	unspecified	kg	-1.515E+05	0	0	-1.515E+05

Figure S47: LCI of basic process

In the characterized impacts per substance (Figure S48) the calculation is the following:

- Carbon dioxide: amountOfCarbonDioxideInLCI *CharacterisationFactorOfCarbonDioxide = -4.319E5*1 = -4.319E5
- Methane: amountOfMethaneInLci*CharacterisationFactorOfMethane = -1.515E5 *25 = -3.787E6



Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**-4.22E+06**
Carbon dioxide, fossil	air	unspecified	-4.319E+05
Methane, fossil	air	unspecified	-3.788E+06

Figure S48: Characterised impacts, per substance, of basic process

In the characterized impacts per process (Figure S49) the details of each subprocess: “test1” and “process-specific emission” are calculated:

- <u>Test1</u>: amountOfCarbonDioxideInLCIPerProcess(Test1)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(Test1)*CharacterisationFactorOfMethane = -4.419E5*1 + (-1.515E5)*25 = -4.229E6
- <u>Process specific emissions</u>: amountOfCarbonDioxideInLciPerProcess(ProcessSpecific)*CharacterisationFactorOfCarbonDioxid

e + amountOfMethaneInLciPerProcess(ProcessSpecific)*CharacterisationFactorOfMethane = 9999*1 + 0*25=1E4

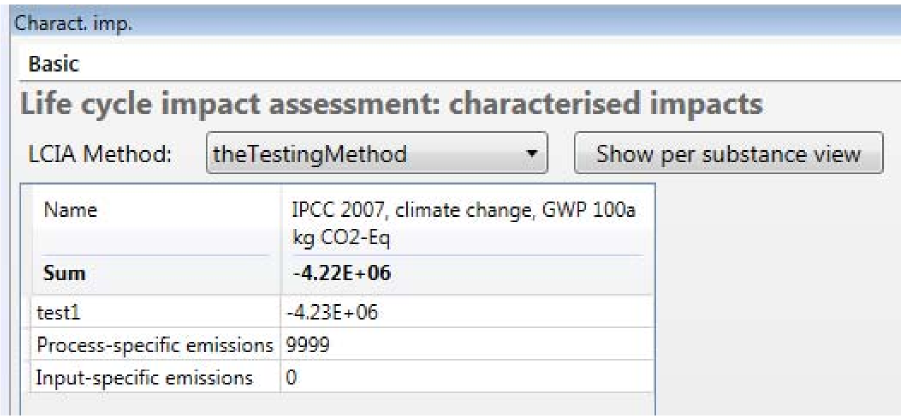


Figure S49: Characterised impacts, per process, of basic process

2.5 Normalised and weighted impacts

The tabs “Norm. imp” and “Weight. Imp.” are very similar to “Charact. Imp.” with the same “per substance” and “per process” views. Figure S50 presents the normalization and weighting factors used.

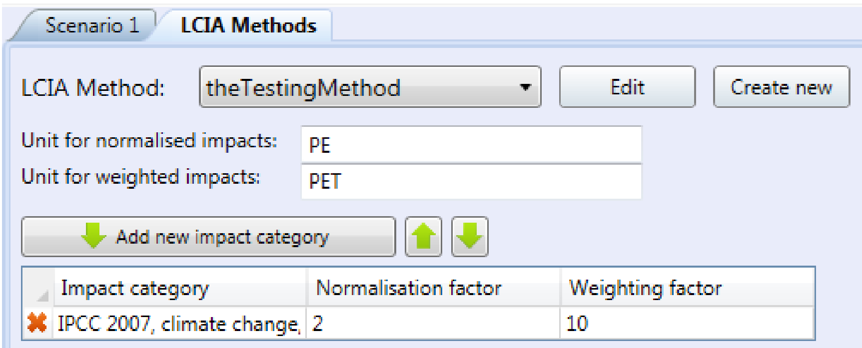


Figure S50: Normalisation and weighting factors used

The normalized impacts are obtained by dividing each number in the characterized impacts by the normalization factor of the impact category.

In the example of the scenario, we calculate based on characterized impact values (Figure S51):

- Carbon dioxide: we had -4.32E5 kg so the normalised impact for the category “IPCC 2007, climate change, GWP 100 a” is: -4.32E5/2 = -2.16E5 PE
- Methane: we had 3.79E6 kg so normalised impact for the category “IPCC 2007, climate change, GWP 100 a” is: -3.79E6 /2 = -1.9E6 PE

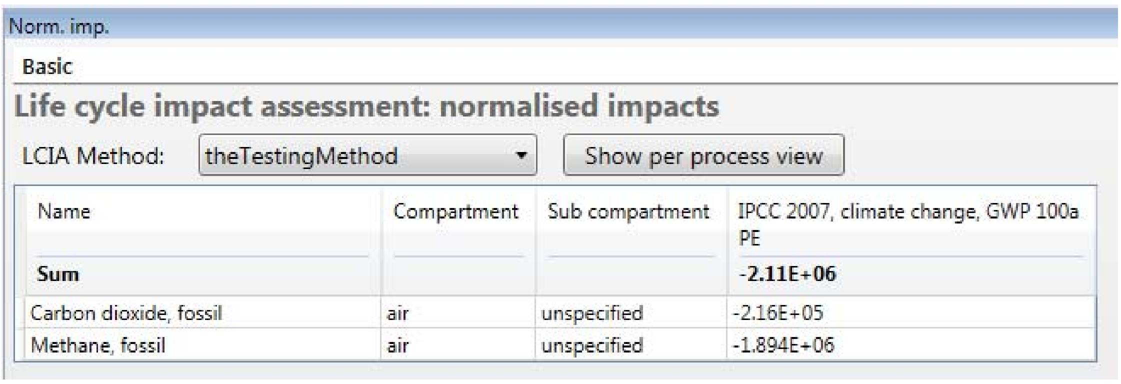


Figure S51: Normalised impacts, per substance, of basic process

And we also divide the characterised impacts in the “per process” view (Figure S52).

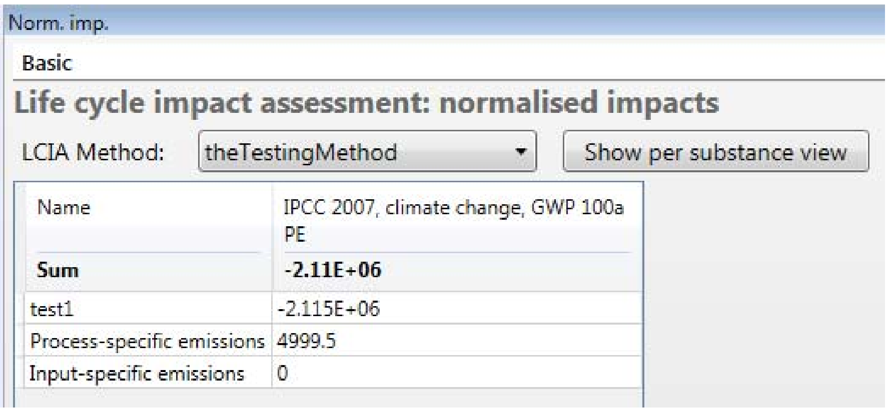


Figure S52: Normalised impacts, per process, of basic process

And the weighted impacts are obtained by <u>multiplying</u> each number in the <u>normalised</u> impacts by the weighting factor of the impact category.

In the example of the scenario, in the normalised imp. per substance view, we had for:

- Carbon dioxide: -2.16E5 kg so the weighted impact for the category “IPCC 2007, climate change, GWP 100 a” is: -2.16E5 *10 = -2.16E6 PE
- Methane: -1.9E6 kg so normalised impact for the category “IPCC 2007, climate change, GWP 100 a” is: -1.9E6 *10 = -1.9E7 PE

Figure S53 and S54 show the weighted impacts, per substance and per process, respectively.

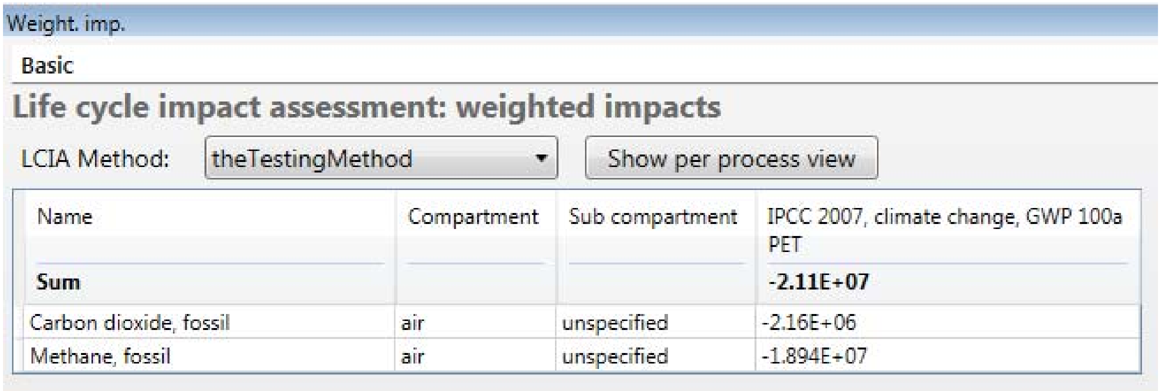


Figure S53: Weighted impacts, per substance, of basic process

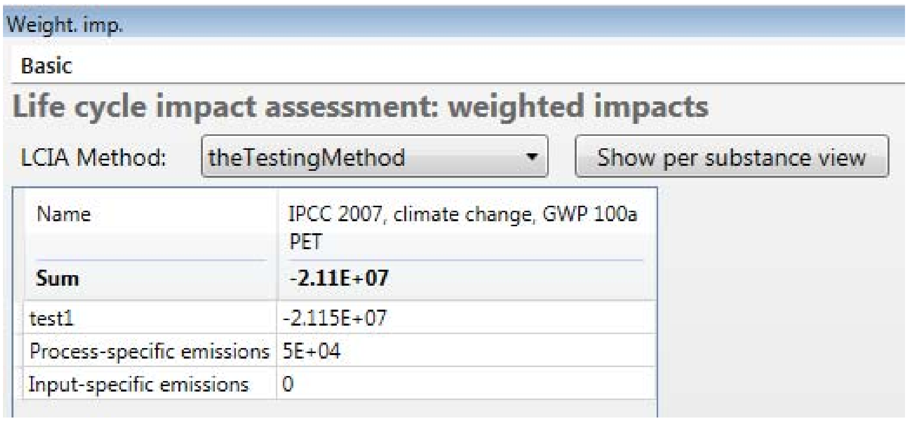


Figure S54: Weighted impacts, per process, of basic process

2.6 Particular case: Material generation

In the material generation process, the user can attach the use of an external process to each material fraction by ticking the tick box "Include upstream impacts" (See Figure S55).

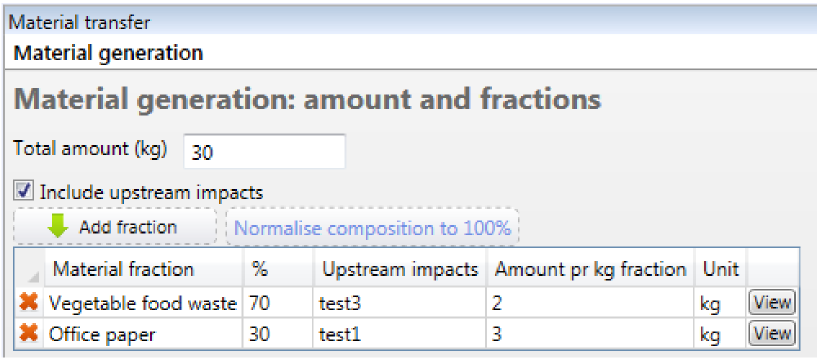


Figure S55: Process exchanges in material generation process

The LCI calculation is for each external process:

LCI = Total_amount *Percentage_field/100 *AmountPerKgFraction *LCI(external_process)

In the example, let's calculate for test3:

- Carbon dioxide: 30 *70/100 *2 *4 = 168 kg
- Methane: 30 *70/100 *2 *2 = 84 kg

And for test1:

- Carbon dioxide: 30 *30/100 *3 *35 = = 945 kg
- Methane: 30 *30/100 *3 *12 = 324 kg

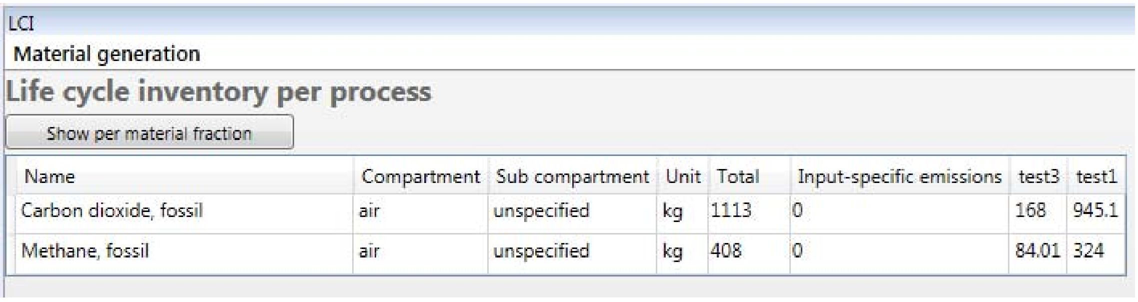


Figure S56: LCI of material generation process

Characterised impact per substance works at process level and at scenario level are calculated as usual by multiplying the total amounts by the characterization factors (Figure S57).

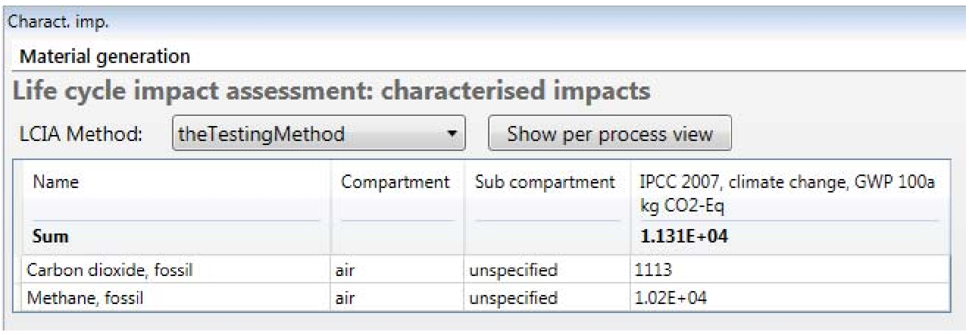


Figure S57: Characterised impact, per substance, of material generation process

Characterised impact per process is calculated by calculating the impact for each external process:

sum_for_each_ele_exch [Total_amount *Percentage_field/100 *AmountPerKgFraction *LCI(external_process) *characterization_factor(elem. exch)]

In our example, we use an impact category with the characterization factor of 1 for "carbon dioxide" and 25 for "methane", so:

- test3: 30 *70/100 *2 *4 *1 + 30 *70/100 *2 *2 *25 = 168*1 + 84*25 =2268
- test1: 30 *30/100 *3 *35 *1 + 30 *30/100 *3 *12 *25 = 945*1 + 324*25 = 9045

So the characterized impacts are as shown in Figure S58 at process level.

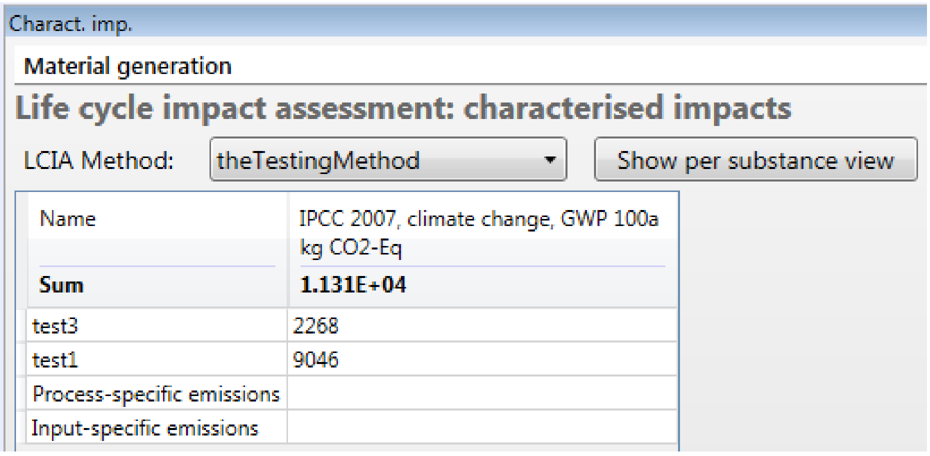


Figure S58: Characterised impact, per process, of material generation process

2.7 Particular case: Energy generation

This process is similar to material generation process except that we need to back-calculate the "Total amount" of input.

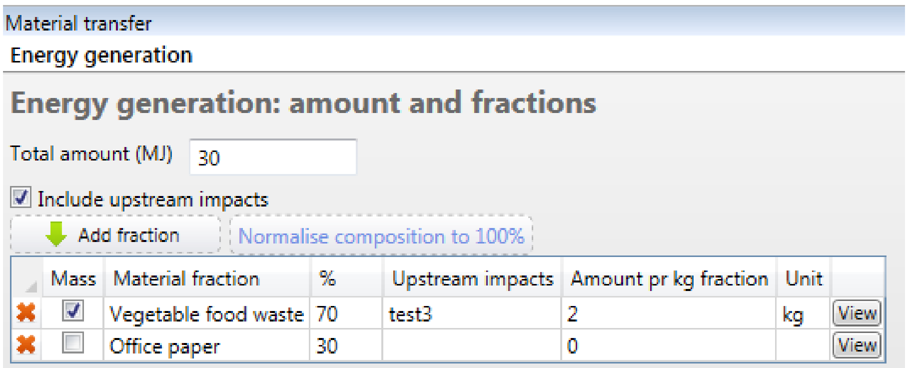


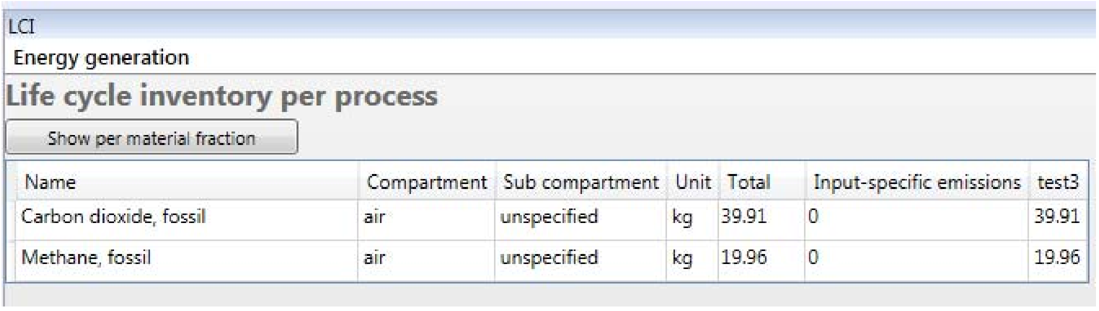
Figure S59: Process exchanges in energy generation process

The LCI calculation is for each external process:

Total_amount(MJ) *Percentage_field(fraction)/100 /energy%(fraction, MJ/kg) *100/TS%(fraction) *AmountPerKgFraction *LCI(external_process)

where energy% and TS% are the properties of the material fraction as found in the library of material fractions.

For vegetable food waste test3 emits: 30 *70/100 /18.3 *100/23 *2 *[4 kg CO2; 2 kg CH4] = [39.91 kg CO2; 19.95 kg CH4]



LCI

Energy generation

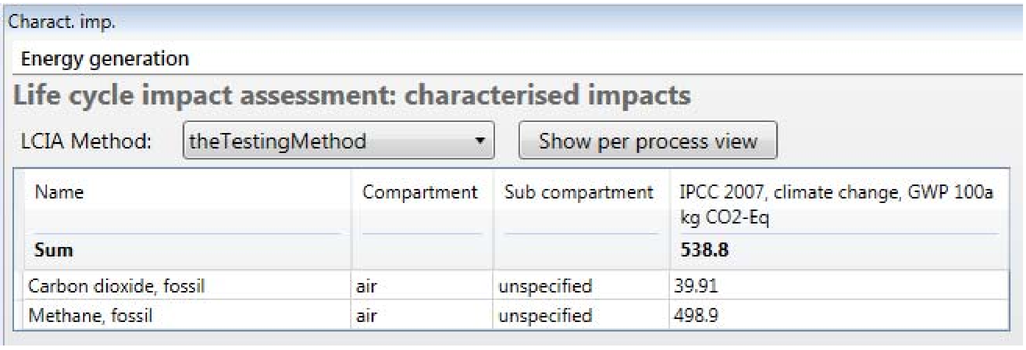
Life cycle inventory per process

Show per material fraction

Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	test3
Carbon dioxide, fossil	air	unspecified	kg	39.91	0	39.91
Methane, fossil	air	unspecified	kg	19.96	0	19.96

Figure S60: LCI of energy generation process

The characterised impacts per substance are for CO2: 39.91 and for CH4: 19.96*25=499.



Charact. imp.

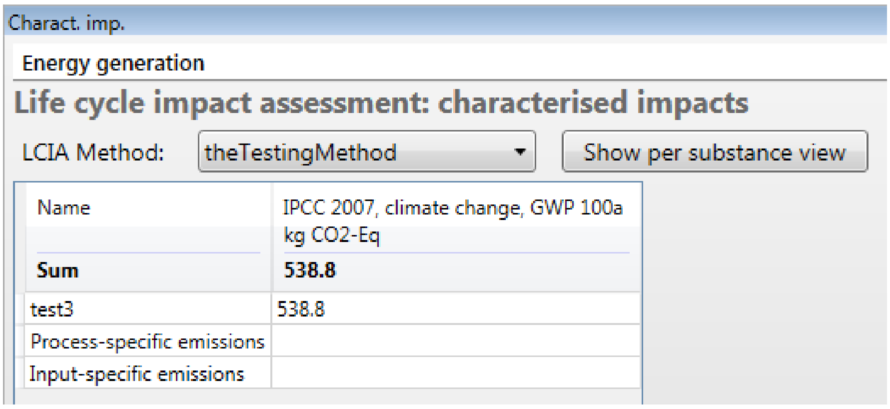
Energy generation

Life cycle impact assessment: characterised impacts

LCIA Method: theTestingMethod | Show per process view

Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**538.8**
Carbon dioxide, fossil	air	unspecified	39.91
Methane, fossil	air	unspecified	498.9

Figure S61: Characterised impact, per substance, of energy generation process



Charact. imp.

Energy generation

Life cycle impact assessment: characterised impacts

LCIA Method: theTestingMethod | Show per substance view

Name	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum	**538.8**
test3	538.8
Process-specific emissions	
Input-specific emissions	

Figure S62: Characterised impact, per process, of energy generation process

3 Input-specific emissions in four material processes

In this section, we explain how the LCI calculations are performed in the material processes templates that include emissions happening in the "Material transfer" tab. These emissions are called "input-specific". Remember that all processes can have "process-specific" emissions due to data in the "Process exchanges" tab (explained in Section I). The 4 processes that can have "input-specific" emissions are:

- Substance transfer per fraction.
- Substance transfer default.
- Use on land.
- Emissions to the environment.

Figure S32 shows the example used where we connect a material generation process each time to a different material process.

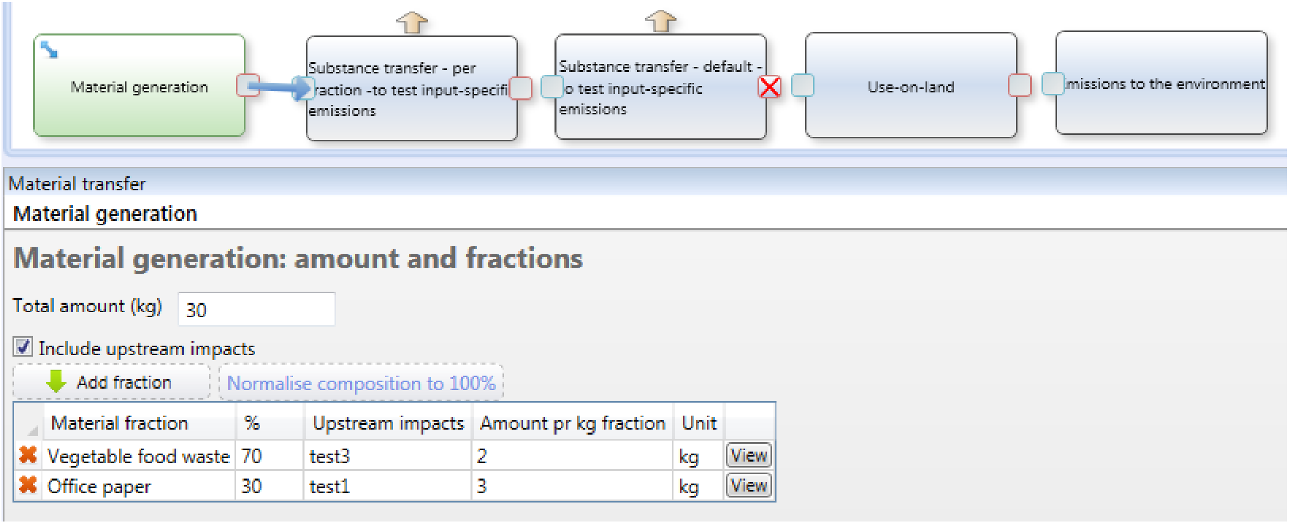


Figure S63: Scenario used to show the calculations of input-specific emissions

This is the composition calculated out of the material generation process.

Fraction name	**Total Wet Weight (kg)**	**TS (kg)**	**Water (kg)**	**VS (kg)**	**Ash (kg)**	**Energy (MJ)**	**C bio (kg)**	**C bio and (kg)**	**C fossil (kg)**	**Ca (kg)**	**Cl (kg)**	**F (kg)**
Vegetable food waste	21	4.83	16.17	4.579	0.2512	88.389	2.294	2.043	0.01154	0.02681	0.02705	0.000483
Office paper	9.005	8.217	0.7875	6.516	1.701	103	3.065	1.693	0.01545	0.6385	0.005752	0.0008217

Fraction name	**H (kg)**	**K (kg)**	**N (kg)**	**Na (kg)**	**O (kg)**	**P (kg)**	**S (kg)**	**Ag (kg)**	**Al (kg)**	**As (kg)**
Vegetable food waste	0.3188	0.06134	0.09177	0.01507	1.908	0.01116	0.008887	0	0.004975	1.265E-06
Office paper	0.4109	0.0009696	0.008217	0.00636	3.016	0.0003139	0.005284	0	0.01076	1.75E-06

3.1 Substance transfer per fraction

Figure S64 shows the added emissions to the “air unspecified” compartment:

- For Cfossil, 2% goes to the air except for the fraction “Vegetable food waste” for which it goes at 15%. Al goes at 40% to the air.
- And we have some process-specific emissions of aluminium and methane, and the use of test3.

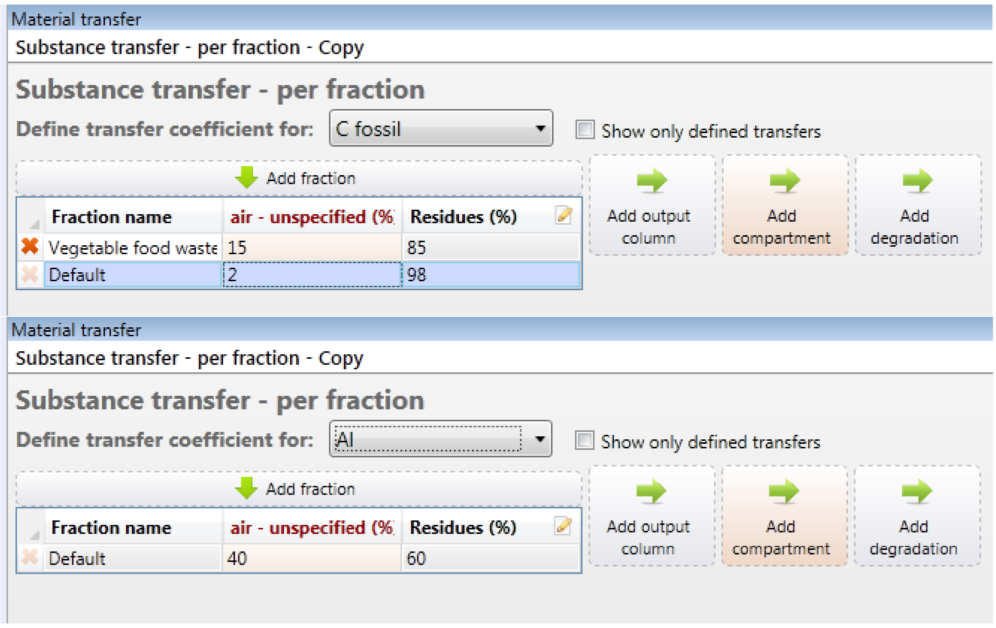


Figure S64: Material transfer for the "substance transfer per fraction" process

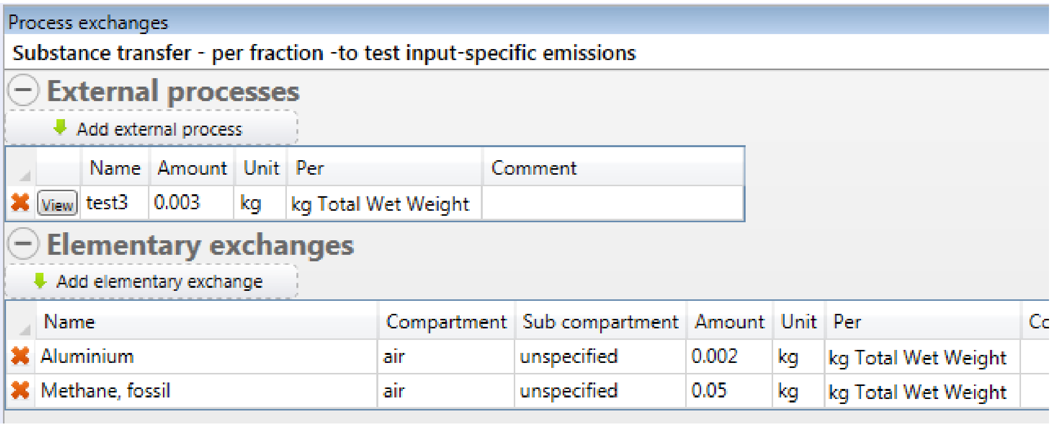


Figure S65: Process exchanges for the "substance transfer per fraction" process

Note that we need an "interface" to explain to EASETECH how Cfossil is emitted: it is emitted as carbon dioxide with a conversion factor of 44/12 (this interface is here by default, just check if you have the right numbers) (see Figure S66).

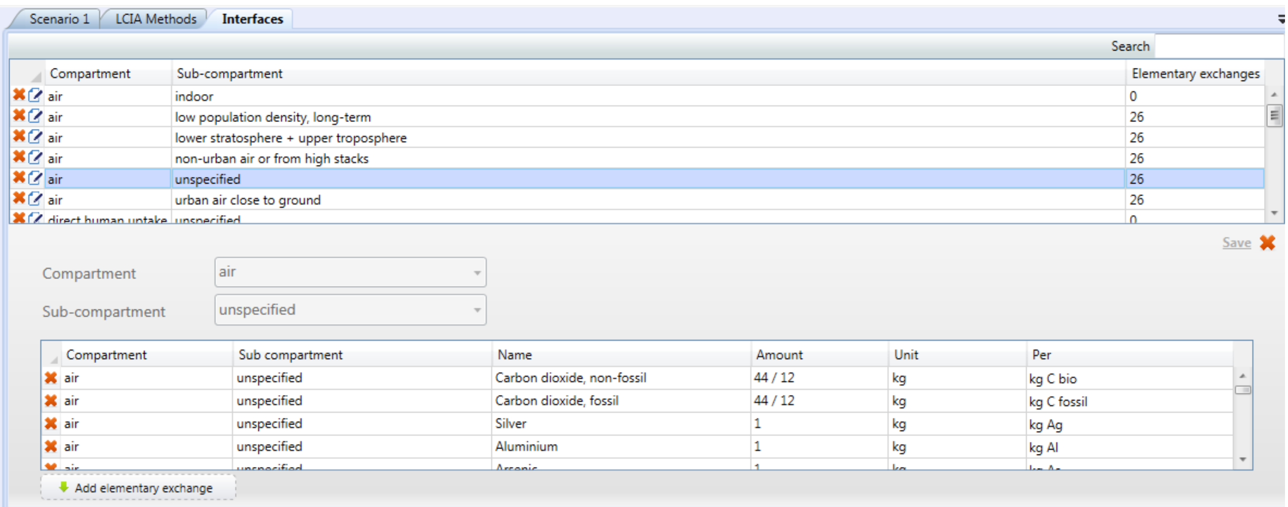


Figure 66: Interface "air – unspecified"

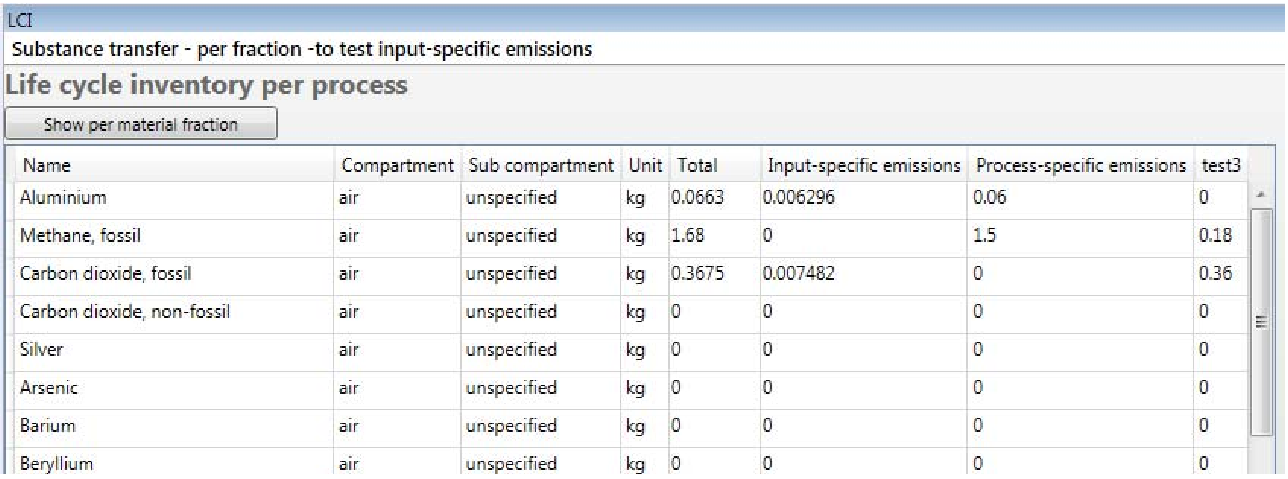
So the LCI of these Material transfer emissions is calculated for each material property in the dropdown list as: SumForAllFractionsOf[TransferCoefficientToCompartment(fraction) *AmountProperty(fraction)] * ConversionFactorInInterface

So in our example:

- Carbon dioxide, air, unspecified: [0.15*input.cfossil(vegetablefoodwaste) + 0.02*input.cfossil(officepaper)] *44/12 = [0.15*0.01154 +0.02*0.01545]*44/12 =0.00748 kg
- Aluminium, air, unspecified: [0.4*input.al(vegetablefoodwaste) + 0.4*input.al (officepaper)] *1 = [0.4*0.004975 +0.4*0.01076]*1 =0.006294 kg

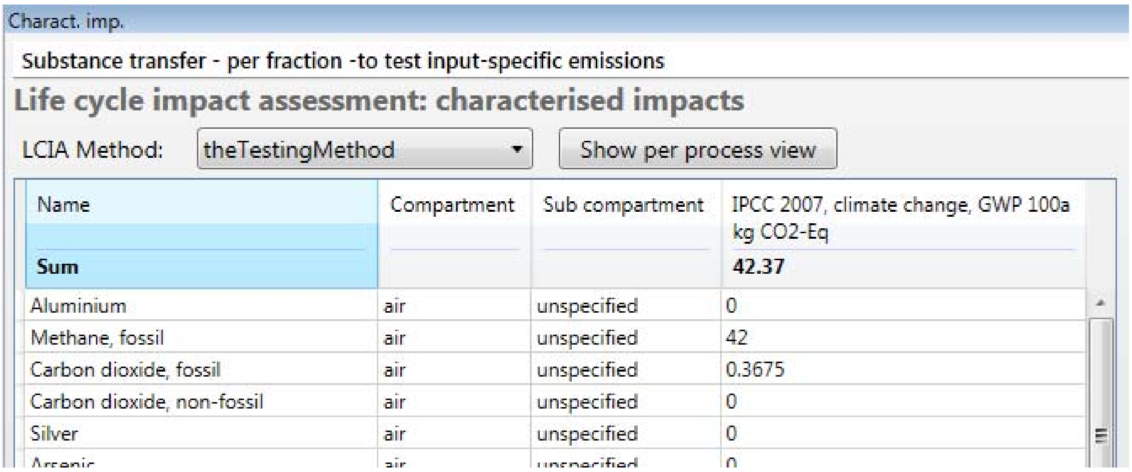
And of course the contributions of the “Process exchanges” tab:

- Process-specific:
  - Aluminium, air, unspecified: 0.002*30=0.06
  - Methane fossil, air, unspecified: 0.05*30=1.5
- Test3: 0.003*30*{2kg CH4; 4 kg CO2} = {0.18 kg CH4; 0.36 kg CO2}.


LCI
Substance transfer - per fraction -to test input-specific emissions
Life cycle inventory per process
Show per material fraction

Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions	test3
Aluminium	air	unspecified	kg	0.0663	0.006296	0.06	0
Methane, fossil	air	unspecified	kg	1.68	0	1.5	0.18
Carbon dioxide, fossil	air	unspecified	kg	0.3675	0.007482	0	0.36
Carbon dioxide, non-fossil	air	unspecified	kg	0	0	0	0
Silver	air	unspecified	kg	0	0	0	0
Arsenic	air	unspecified	kg	0	0	0	0
Barium	air	unspecified	kg	0	0	0	0
Beryllium	air	unspecified	kg	0	0	0	0

Figure S67: LCI of the “substance transfer per fraction” process


Charact. imp.
Substance transfer - per fraction -to test input-specific emissions
Life cycle impact assessment: characterised impacts
LCIA Method: theTestingMethod
Show per process view

Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**42.37**
Aluminium	air	unspecified	0
Methane, fossil	air	unspecified	42
Carbon dioxide, fossil	air	unspecified	0.3675
Carbon dioxide, non-fossil	air	unspecified	0
Silver	air	unspecified	0
Arsenic	air	unspecified	0

Figure S68: Characterised impacts (subs) of the “substance transfer per fraction” process

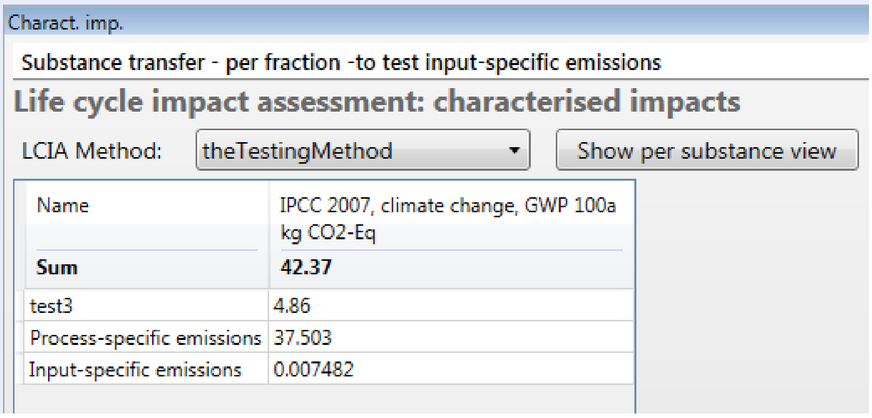


Figure S69: Characterised impacts (process) of the "substance transfer per fraction" process

3.2 Substance transfer default

We implement the same values as in "substance transfer per fraction" into a new process based on template "substance transfer default". The only difference is that in this process the user cannot specify different transfer coefficients for different material fractions.

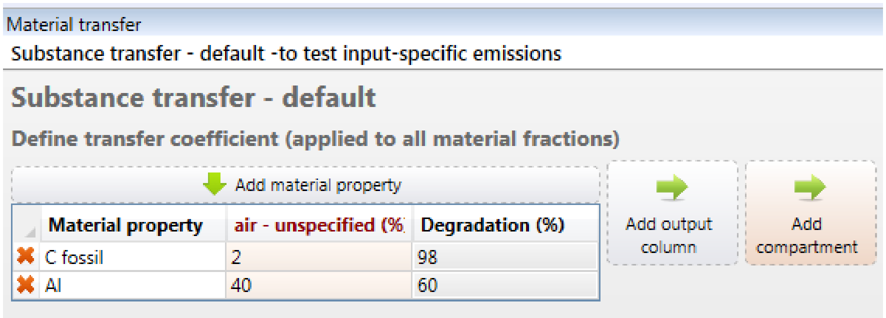


Figure S70: Material transfer for the "substance transfer default" process

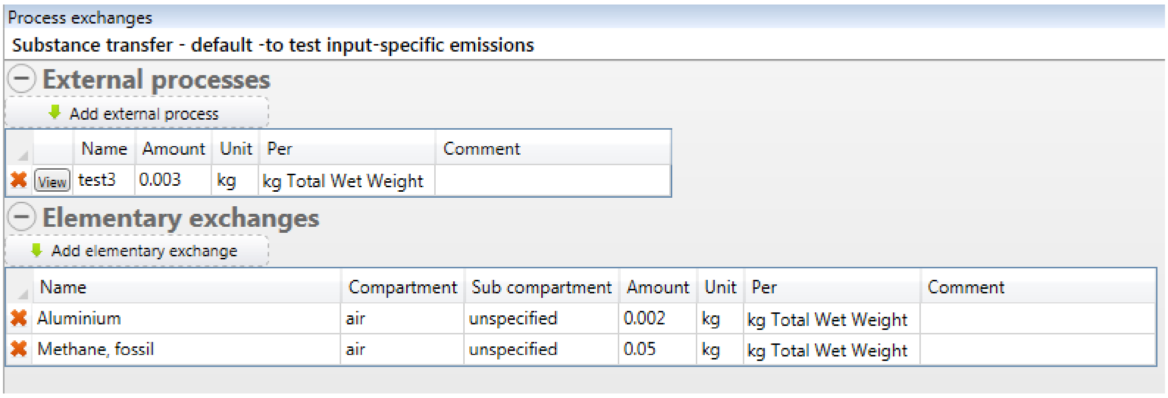


Figure S71: Process exchanges for the "substance transfer default" process

The calculation of characterised impacts also relies on the interfaces.

Very similarly to "substance transfer per fraction", the LCI of these input-specific emissions is calculated for each material property in the dropdown list as: TransferCoefficientToCompartment * SumForAllFractionsOf (AmountProperty) * ConversionFactorInInterface

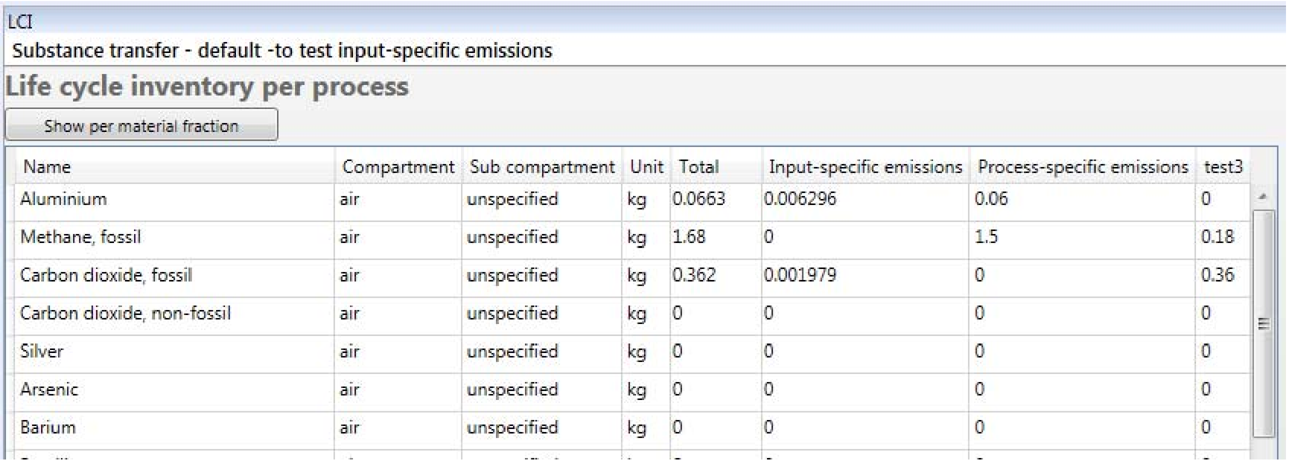
So in our example:

- Carbon dioxide, air, unspecified: 0.02*(input.cfossil(vegetablefoodwaste) + input.cfossil(officepaper)] *44/12 = 0.02* (0.01154 +0.01545]*44/12 =0.001979 kg

- Aluminium, air, unspecified: 0.4* (input.al(vegetablefoodwaste) + input.al (officepaper)] *1 = 0.4*[0.004975 +0.01076]*1 =0.006294 kg

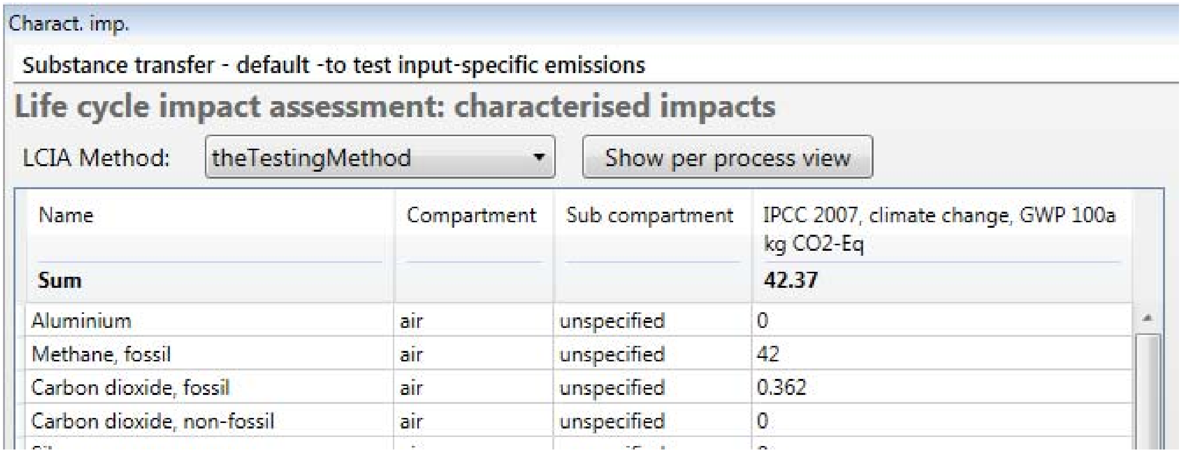
And the contributions of the "process exchange" tab:

- Process-specific:
  - o Aluminium, air, unspecified: 0.002*30=0.06
  - o Methane fossil, air, unspecified: 0.05*30=1.5
- Test3: 0.003*30*{2kg CH4; 4 kg CO2} = {0.18 kg CH4; 0.36 kg CO2}.



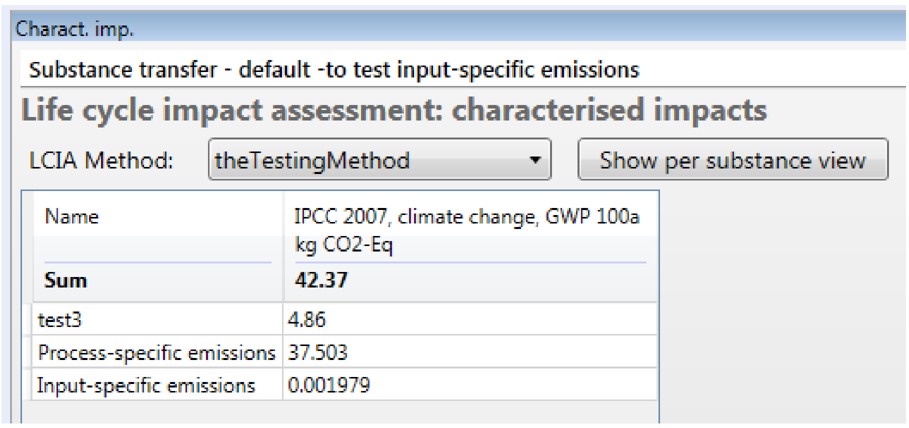
Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions	test3
Aluminium	air	unspecified	kg	0.0663	0.006296	0.06	0
Methane, fossil	air	unspecified	kg	1.68	0	1.5	0.18
Carbon dioxide, fossil	air	unspecified	kg	0.362	0.001979	0	0.36
Carbon dioxide, non-fossil	air	unspecified	kg	0	0	0	0
Silver	air	unspecified	kg	0	0	0	0
Arsenic	air	unspecified	kg	0	0	0	0
Barium	air	unspecified	kg	0	0	0	0

Figure S72: LCI of the "substance transfer default" process



Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**42.37**
Aluminium	air	unspecified	0
Methane, fossil	air	unspecified	42
Carbon dioxide, fossil	air	unspecified	0.362
Carbon dioxide, non-fossil	air	unspecified	0

Figure S73: Characterised impacts (subs) of the "substance transfer default" process



Name	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum	**42.37**
test3	4.86
Process-specific emissions	37.503
Input-specific emissions	0.001979

Figure S74: Characterised impacts (process) of the "substance transfer default" process

3.3 Use on land (UOL)

The material transfer tab of the UOL process contains all data to calculate the "input-specific" emissions. "Input-specific emissions" is the sub-process of all emissions coming from data in the Material transfer tab. As explained in Section I, "process-specific emissions" are elementary exchanges in the "Process exchanges" tab and each external process used is a subprocess as well.

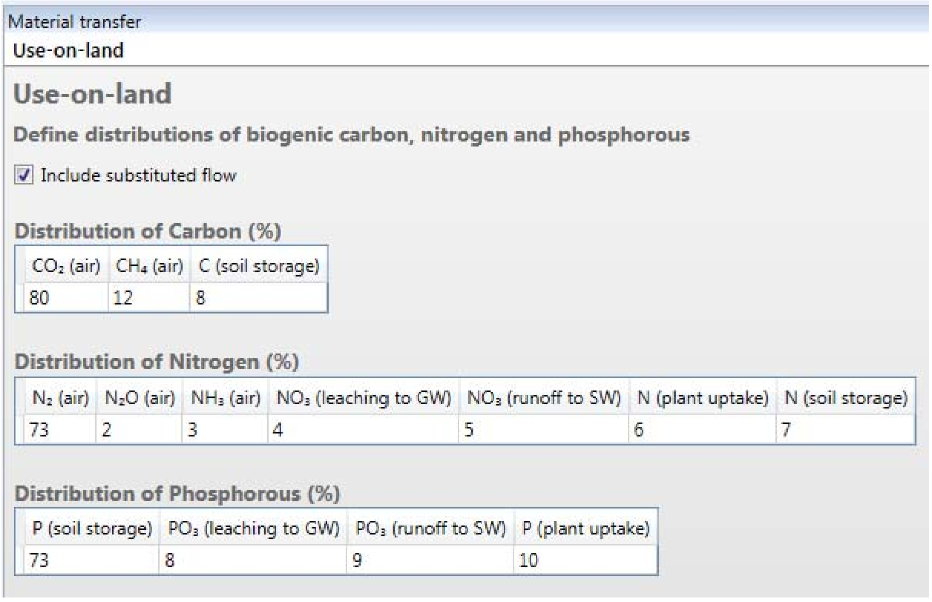


Figure S75: Material transfer for the UOL process

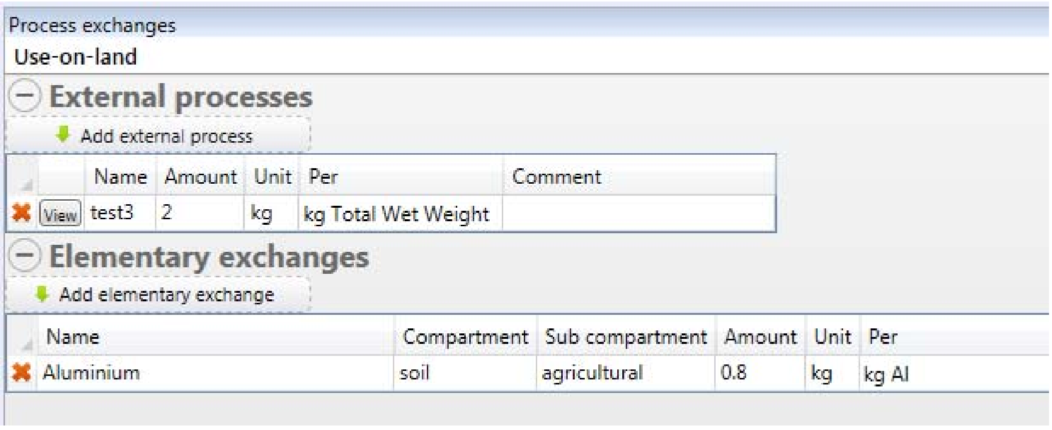


Figure S76: Process exchanges for the UOL process

If I call a, b, c, d...n the values input in the 3 tables in the material transfer tab of UOL, the following input-specific emissions have to be included in the LCI:

- "Carbon dioxide, non-fossil, air, unspecified": input.cbio * a/100 *(2*M_O+M_C)/M_C
- "Methane, non-fossil, air, unspecified": input.cbio * b/100 *(4*M_H+M_C)/M_C
- "Carbon dioxide, fossil, air, unspecified" = input.cbio * c/ 100 *(2*M_O+M_C)/M_C * (-1)
- "Dinitrogen monoxide, air, unspecified": input.n * e/100 *(2*M_N+M_O)/(2*M_N)
- "Ammonia, air, unspecified": input.n * f/100 *(3*M_H+M_N)/M_N
- "Nitrates, water, ground-": input.n * g/100 *(3*M_O+M_N)/M_N
- "Nitrates, water, surface water": input.n * h/100 *(3*M_O+M_N)/M_N
- "Phosphate, water, ground-": input.p * l/100 *(3*M_O+M_P)/M_P
- "Phosphate, water, surface water": input.p * m/100 *(3*M_O+M_P)/M_P

Note that M_C, M_O, M_P and M_H are constants of the catalogue of constants and they are the molar masses of carbon, oxygen, phosphorous and hydrogen.

So the LCI of the subprocess "Input-specific" is calculated in the example like this:

- "Carbon dioxide, non-fossil, air, unspecified": (2.294+3.065) * 80/100 *(2*15.999+12.011)/12.011 =15.71 kg
- "Methane, non-fossil, air, unspecified": (2.294+3.065)* 12/100 *(4*1.008+12.011)/ 12.011 =0.859 kg
- "Carbon dioxide, fossil, air, unspecified" = (2.294+3.065)* 8/ 100 *(2*15.999+12.011)/ 12.011* (-1) =-1.57 kg
- "Dinitrogen monoxide, air, unspecified": (0.09177+0.008217) * 2/100 *(2*14.007+15.999) /(2*14.007) =0.00314 kg
- "Ammonia, air, unspecified": (0.09177+0.008217) * 3/100 *(3*1.008+14.007)/ 14.007 =0.00364 kg
- "Nitrates, water, ground-": (0.09177+0.008217) * 4/100 *(3*15.999+14.007)/ 14.007 =0.0177 kg
- "Nitrates, water, surface water": (0.09177+0.008217) * 5/100 *(3*15.999+14.007)/ 14.007 =0.0221 kg
- "Phosphate, water, ground-": (0.01116+0.0003139) * 8/100 *(3*15.999+30.974)/ 30.974 =0.00234 kg
- "Phosphate, water, surface water": (0.01116+0.0003139) * 9/100 *(3*15.999+30.974)/ 30.974 =0.00263 kg

The process "test3" has also emissions as explained in part I: 2*30*{4kg CO_2; 2kgCH_4} ={240 kg CO_2; 120 kg CH_4}.

And in "Process-specific emissions", we have one emission of aluminium of 0.8 kg/kg Al = 0.8*(0.004975+0.01076) = 0.01259 kg.

LCI

Use-on-land

Life cycle inventory per process

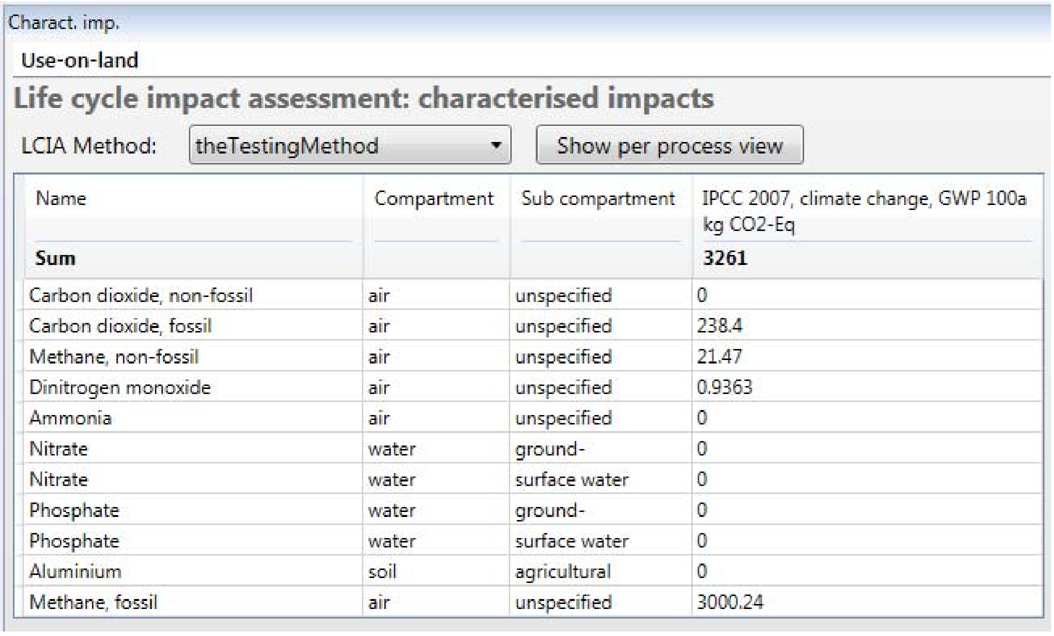
Show per material fraction

Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions	test3
Carbon dioxide, non-fossil	air	unspecified	kg	15.71	15.71	0	0
Carbon dioxide, fossil	air	unspecified	kg	238.4	-1.571	0	240
Methane, non-fossil	air	unspecified	kg	0.859	0.859	0	0
Dinitrogen monoxide	air	unspecified	kg	0.003142	0.003142	0	0
Ammonia	air	unspecified	kg	0.003647	0.003647	0	0
Nitrate	water	ground-	kg	0.0177	0.0177	0	0
Nitrate	water	surface water	kg	0.02213	0.02213	0	0
Phosphate	water	ground-	kg	0.00234	0.00234	0	0
Phosphate	water	surface water	kg	0.002632	0.002632	0	0
Aluminium	soil	agricultural	kg	0.01259	0	0.01259	0
Methane, fossil	air	unspecified	kg	120	0	0	120

Figure S77: LCI of the UOL process

For characterised impacts per substance, let's look only at the impact category "Climate change" that has characterisation factors for "carbon dioxide, fossil, air" of 1, for "Methane, air" of 25, for "dinitrogen monoxide" of 293:

- Carbon dioxide, fossil: amountOfCarbonDioxideFossilInLCI*CharacterisationFactorOfCarbonDioxide =238.4*1 =238.4
- Methane, fossil: amountOfMethaneFossilInLCI*CharacterisationFactorOfMethane =120*25=3000
- Methane, non-fossil: amountOfMethaneNonFossilInLCI*CharacterisationFactorOfMethane =0.859*25=21.47 kg
- Dinitrogen monoxide: amountOfDinitrogenMonoxideInLCI*CharacterisationFactorOfDinitrogenMonoxide =0.003142*298=0.9363 kg



Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**3261**
Carbon dioxide, non-fossil	air	unspecified	0
Carbon dioxide, fossil	air	unspecified	238.4
Methane, non-fossil	air	unspecified	21.47
Dinitrogen monoxide	air	unspecified	0.9363
Ammonia	air	unspecified	0
Nitrate	water	ground-	0
Nitrate	water	surface water	0
Phosphate	water	ground-	0
Phosphate	water	surface water	0
Aluminium	soil	agricultural	0
Methane, fossil	air	unspecified	3000.24

Figure S78: Characterised impacts (subs) of the UOL process

In the characterized impacts per process the details of each subprocess: “test3”, “process-specific emission” are calculated:

- For the subprocess “test3”: amountOfCarbonDioxideInLCIPerProcess(Test3)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(Test3)*CharacterisationFactorOfMethane = 240*1 + 120*25 =3240 kg
- For Process-specific emissions: amountOfCarbonDioxideFossilInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfMethane + amountOfDinitrogenMonoxideInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfDinitrogenMonoxide
  = -1.571*1 + 0.859*25 +0.003142*298 =20.84 kg

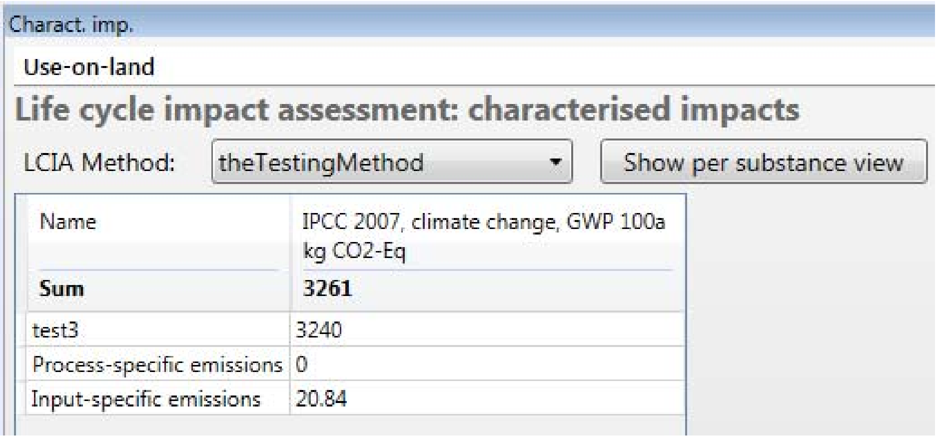


Figure S79: Characterised impacts (process) of the UOL process

3.4 Emissions to the environment

This process has also a material transfer tab that creates input-specific emissions. In the example following we see that 2 emissions are coming from the "Material transfer" tab (input-specific emission), while one is coming from the "Process exchanges" tab (process-specific emission) and we use one external process. So we have 3 sub-processes.

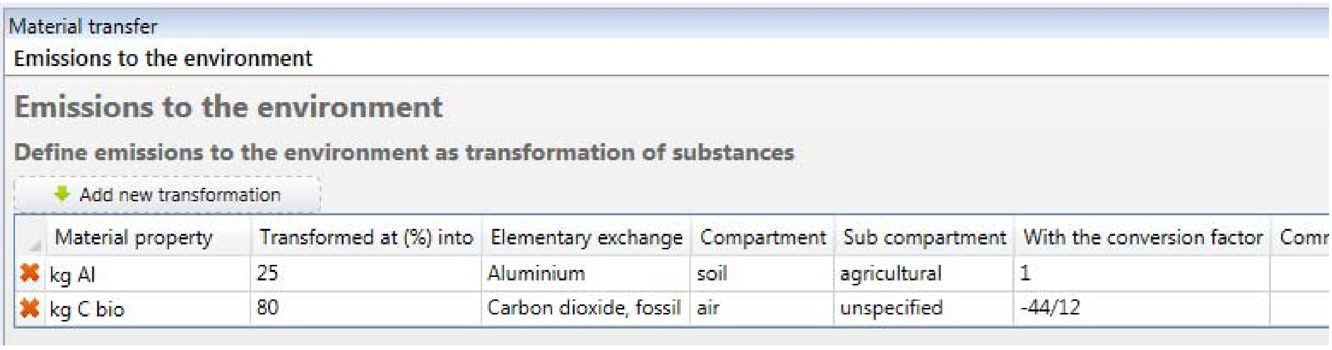


Figure S80: Material transfer for the Emissions to the environment process

Figure S81: Process exchanges for the Emissions to the environment process

The LCI of the emissions happening in the material transfer is calculated for each line as amountOfPropertyInInput *TransformedAtPercent/100 *ConversionFactor

So for our two emissions, it gives:

- Carbon dioxide, fossil, air, unspecified : input.Cbio*80/100*(-44/12) = -15.72 kg
- Aluminium, soil, agricultural: input.Al*25/100*1=0.003935 kg

For the other emissions, it happens as explained in part I: we have an (additional) emission of aluminium of 0.02*30=0.6 kg and emissions from test3 of 2*30*{2kg CH4; 4 kg CO2} = {120 kg CH4; 240 kg CO2}.

LCI

Emissions to the environment

Life cycle inventory per process

Show per material fraction

Name	Compartment	Sub compartment	Unit	Total	Input-specific emissions	Process-specific emissions	test3
Aluminium	soil	agricultural	kg	0.604	0.003935	0.6	0
Carbon dioxide, fossil	air	unspecified	kg	224.3	-15.72	0	240
Methane, fossil	air	unspecified	kg	120	0	0	120

Figure S82: LCI of the Emissions to the environment process

The "characterised impact per substance" tab shows as usual for each elementary exchange, the total amount multiplied by the characterisation factor.

Charact. imp.

Emissions to the environment

Life cycle impact assessment: characterised impacts

LCIA Method: theTestingMethod | Show per process view

Name	Compartment	Sub compartment	IPCC 2007, climate change, GWP 100a kg CO2-Eq
Sum			**3225**
Aluminium	soil	agricultural	0
Carbon dioxide, fossil	air	unspecified	224.3
Methane, fossil	air	unspecified	3000.24

Figure S83: Characterised impacts (subs) of the Emissions to the environment process

And the characterised impact per process shows for each subprocess, the sum for all elementary exchanges of amount multiplied by characterisation factor:

- For the subprocess "test3": amountOfCarbonDioxideInLCIPerProcess(Test3)*CharacterisationFactorOfCarbonDioxide + amountOfMethaneInLCIPerProcess(Test3)*CharacterisationFactorOfMethane = 240*1 + 120*25 =3240 kg
- For **input-specific** emissions: amountOfCarbonDioxideFossilInLCIPerProcess(ProcessSpecific)*CharacterisationFactorOfCarbonDioxide = -15.72*1 = -15.72 kg

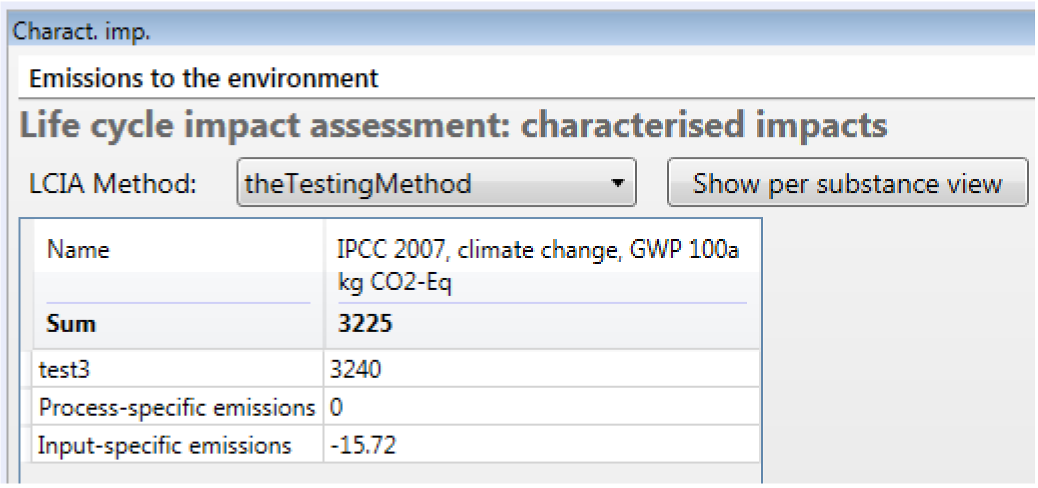


Figure S84: Characterised impacts (process) of the Emissions to the environment process

PART IV: CASE STUDY

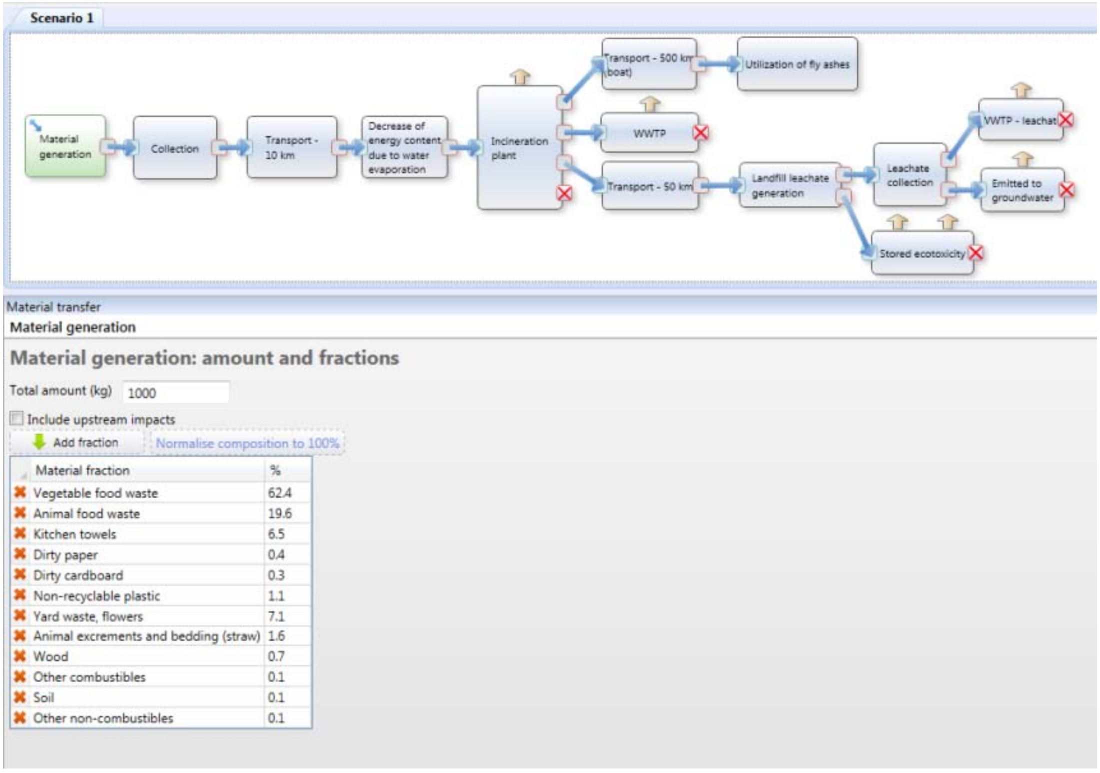
In this document are presented screenshots of how the systems were implemented in EASETECH. Please refer to the original paper by Clavreul et al. (2012) for further details.

1 Scenario construction and data input

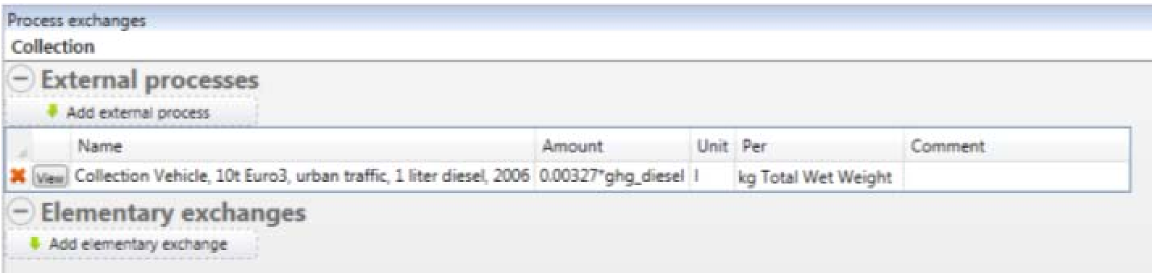
The name of the template used to build each module is provided, as well as screenshots showing the data. Note that parameters were used in some number fields, there value is given in the Section 3 of this Part III.

1.1 Incineration scenario

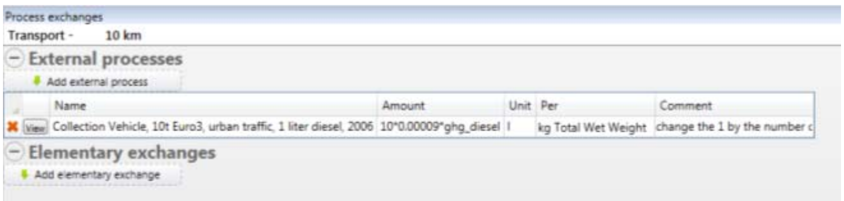
Material generation, based on “Material generation” template:



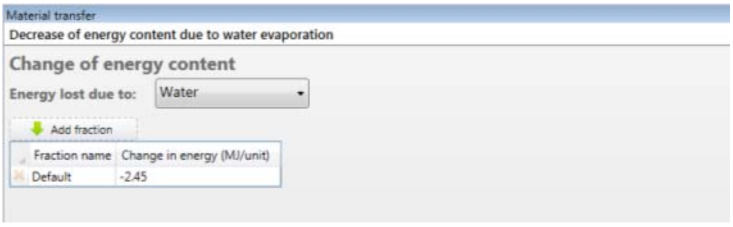
Collection, based on the “Basic process” template:



Transport, based on the “Basic process” template:



Decrease of energy content due to water evaporation, based on the “Change of energy content” template:


Material transfer
Decrease of energy content due to water evaporation

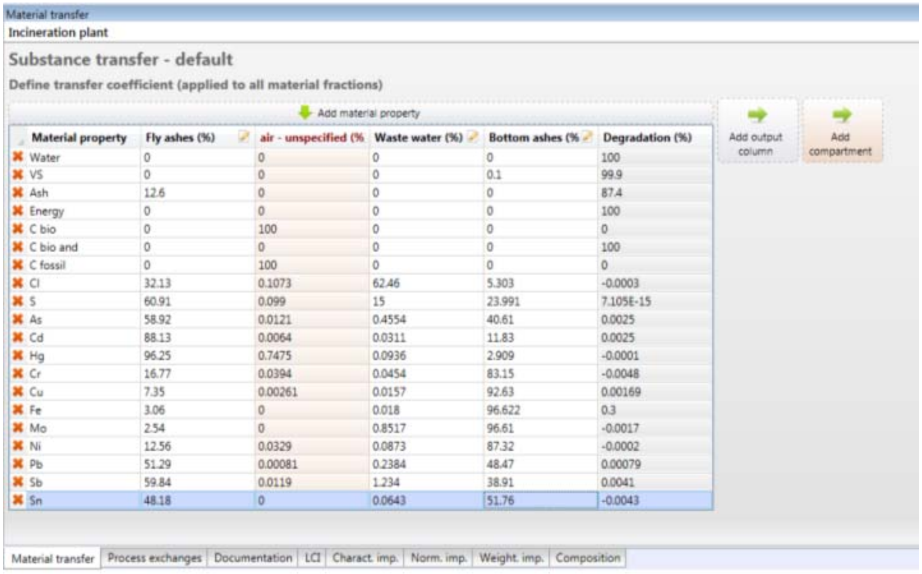
Change of energy content

Energy lost due to: Water

Add fraction

Fraction name	Change in energy (MJ/unit)
Default	-2.45

Incineration plant, based on the “Substance transfer, default” template (note that the template “Substance transfer, per fraction” could have been used instead offering the possibility of giving different values to different material fractions):


Material transfer
Incineration plant

Substance transfer - default

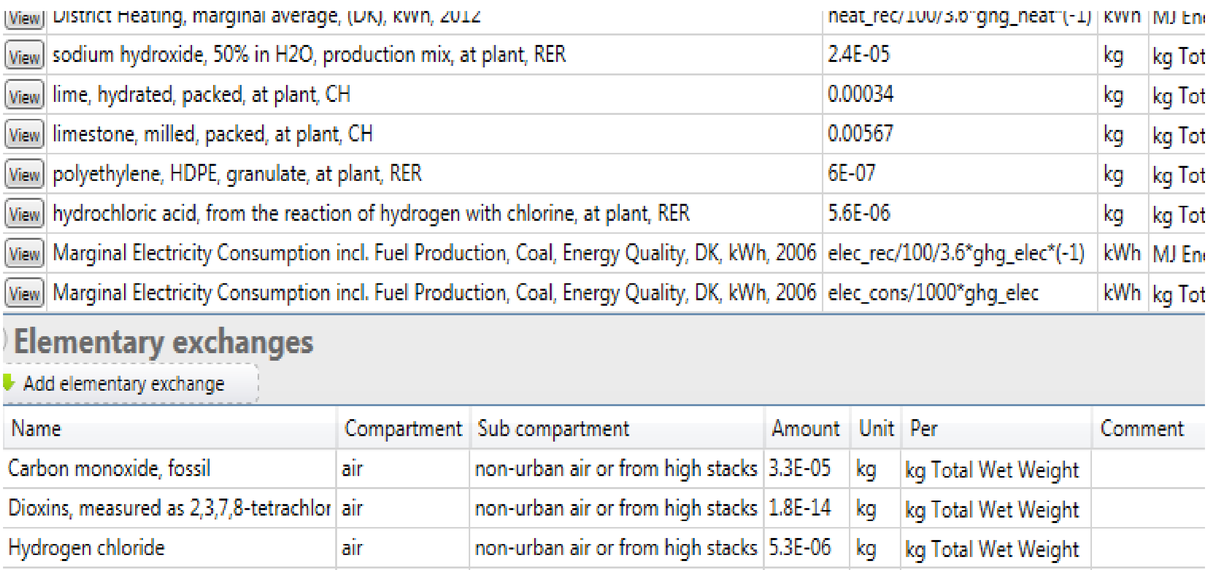
Define transfer coefficient (applied to all material fractions)

Add material property

Material property	Fly ashes (%)	air - unspecified (%	Waste water (%)	Bottom ashes (%	Degradation (%)
Water	0	0	0	0	100
VS	0	0	0	0.1	99.9
Ash	12.6	0	0	0	87.4
Energy	0	0	0	0	100
C bio	0	100	0	0	0
C bio and	0	0	0	0	100
C fossil	0	100	0	0	0
Cl	32.13	0.1073	62.46	5.303	-0.0003
S	60.91	0.099	15	23.991	7.105E-15
As	58.92	0.0121	0.4554	40.61	0.0025
Cd	88.13	0.0064	0.0311	11.83	0.0025
Hg	96.25	0.7475	0.0936	2.909	-0.0001
Cr	16.77	0.0394	0.0454	83.15	-0.0048
Cu	7.35	0.00261	0.0157	92.63	0.00169
Fe	3.06	0	0.018	96.622	0.3
Mo	2.54	0	0.8517	96.61	-0.0017
Ni	12.56	0.0329	0.0873	87.32	-0.0002
Pb	51.29	0.00081	0.2384	48.47	0.00079
Sb	59.84	0.0119	1.234	38.91	0.0041
Sn	48.18	0	0.0643	51.76	-0.0043

Add output column
Add compartment

Material transfer | Process exchanges | Documentation | LCI | Charact. imp. | Norm. imp. | Weight. imp. | Composition



View	District Heating, marginal average, (DK), kWh, 2012	heat_rec/100/3.6*ghg_heat*(-1)	kWh	MJ En
View	sodium hydroxide, 50% in H2O, production mix, at plant, RER	2.4E-05	kg	kg Tot
View	lime, hydrated, packed, at plant, CH	0.00034	kg	kg Tot
View	limestone, milled, packed, at plant, CH	0.00567	kg	kg Tot
View	polyethylene, HDPE, granulate, at plant, RER	6E-07	kg	kg Tot
View	hydrochloric acid, from the reaction of hydrogen with chlorine, at plant, RER	5.6E-06	kg	kg Tot
View	Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	elec_rec/100/3.6*ghg_elec*(-1)	kWh	MJ En
View	Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	elec_cons/1000*ghg_elec	kWh	kg Tot

Elementary exchanges

Add elementary exchange

Name	Compartment	Sub compartment	Amount	Unit	Per	Comment
Carbon monoxide, fossil	air	non-urban air or from high stacks	3.3E-05	kg	kg Total Wet Weight	
Dioxins, measured as 2,3,7,8-tetrachlor	air	non-urban air or from high stacks	1.8E-14	kg	kg Total Wet Weight	
Hydrogen chloride	air	non-urban air or from high stacks	5.3E-06	kg	kg Total Wet Weight	

Transport 500 km (boat), based on the “Basic process” template:

Process exchanges

Transport - 500 km (boat)

External processes

Add external process

Name	Amount	Unit	Per	Comment
Bulk carrier ocean; technology mix; 100.000-200.000 dwt, ELCD, 2005	0.00569*1.76e5*500*1e-3	kg*km	kg Total Wet Weight	0.00569*1.76e-5 kgkm /km/tc

Elementary exchanges

Add elementary exchange

Utilisation of fly ashes, based on the "Basic process" template:

Process exchanges

Utilization of fly ashes

External processes

Add external process

Name	Amount	Unit	Per	Comment
limestone, milled, packed, at plant, CH	-0.035	kg	kg Total Wet Weight	substituted due to alkalinity of the residues
Production and Combustion of Diesel Oil in Truck, EU2, 1998	0.0006	kg	kg Total Wet Weight	Used for mixing the residues and pumping them to quarry
Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	0.013*ghg_elec	kWh	kg Total Wet Weight	Used for mixing the residues and pumping them to quarry

Elementary exchanges

Add elementary exchange

Name	Compartment	Sub compartment	Amount	Unit	Per	Comment
Lead	water	surface water	3.1E-10	kg	kg Total Wet Weight	Waste water emissions from quarry
Mercury	water	surface water	6.1E-11	kg	kg Total Wet Weight	Waste water emissions from quarry
Sulfate	water	surface water	0.00082	kg	kg Total Wet Weight	Waste water emissions from quarry
Chloride	water	surface water	0.0092	kg	kg Total Wet Weight	Waste water emissions from quarry
Zinc, ion	water	surface water	1.4E-08	kg	kg Total Wet Weight	Waste water emissions from quarry
Nickel, ion	water	surface water	1.5E-09	kg	kg Total Wet Weight	Waste water emissions from quarry
Thallium	water	surface water	4.1E-10	kg	kg Total Wet Weight	Waste water emissions from quarry
Cadmium, ion	water	surface water	3.1E-09	kg	kg Total Wet Weight	Waste water emissions from quarry

Waste water treatment plant, based on the "Substance transfer - default" template:

Material transfer

WWTP

Substance transfer - default

Define transfer coefficient (applied to all material fractions)

Add material property | Add output column | Add compartment

Material property	water - surface wat	Degradation (%)
Ca	15	85
Cl	15	85
K	15	85
Na	15	85
P	15	85
S	15	85
Al	15	85
As	30	70
Cd	15	85
Cr	70	30
Cu	50	50
Fe	15	85
Hg	15	85
Mg	15	85
Mn	15	85
Mo	15	85
Ni	15	85
Pb	15	85
Sb	15	85
Sn	15	85
Zn	30	70

Process exchanges

WWTP

External processes

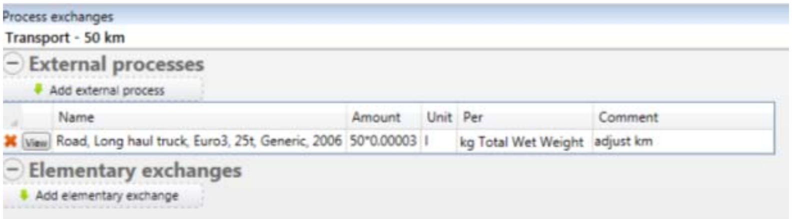
Add external process

Name	Amount	Unit	Per	Comment
Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	0.004	kWh	kg Total Wet Weight	

Elementary exchanges

Add elementary exchange

Transport – 50 km, based on the "Basic process" template:


Process exchanges

Transport - 50 km

External processes

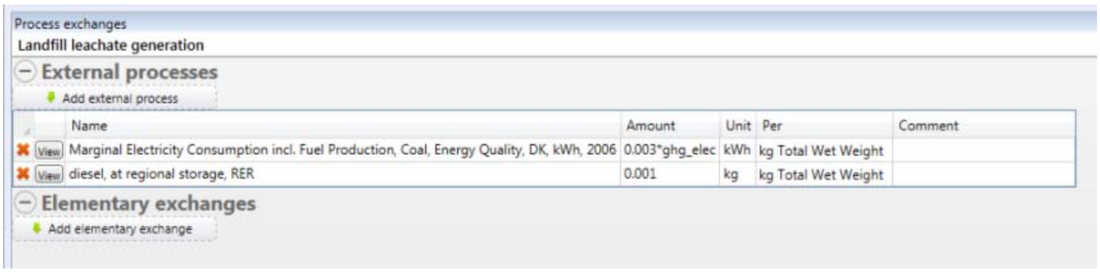
Add external process

Name	Amount	Unit	Per	Comment
Road, Long haul truck, Euro3, 25t, Generic, 2006	50*0.00003	l	kg Total Wet Weight	adjust km

Elementary exchanges

Add elementary exchange

Landfill leachate generation, based on the “Leachate generation” template:


Process exchanges

Landfill leachate generation

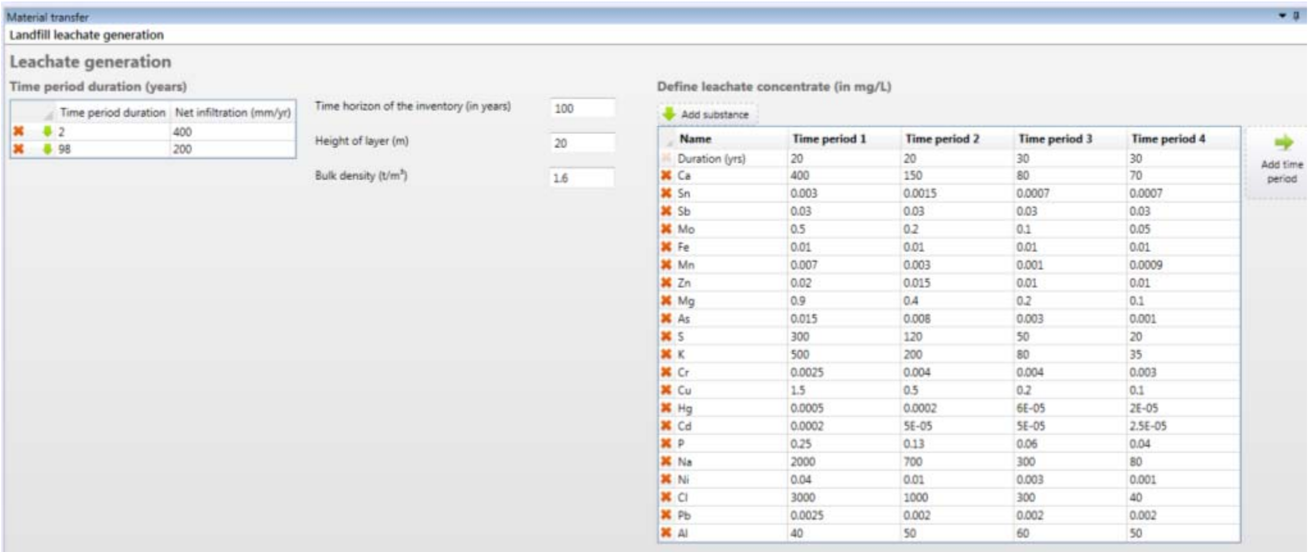
External processes

Add external process

Name	Amount	Unit	Per	Comment
Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	0.003*ghg_elec	kWh	kg Total Wet Weight	
diesel, at regional storage, RER	0.001	kg	kg Total Wet Weight	

Elementary exchanges

Add elementary exchange


Material transfer

Landfill leachate generation

Leachate generation

Time period duration (years)

Time period duration	Net infiltration (mm/yr)
2	400
98	200

Time horizon of the inventory (in years): 100

Height of layer (m): 20

Bulk density (t/m³): 1.6

Define leachate concentrate (in mg/L)

Add substance

Name	Time period 1	Time period 2	Time period 3	Time period 4
Duration (yrs)	20	20	30	30
Ca	400	150	80	70
Sn	0.003	0.0015	0.0007	0.0007
Sb	0.03	0.03	0.03	0.03
Mo	0.5	0.2	0.1	0.05
Fe	0.01	0.01	0.01	0.01
Mn	0.007	0.003	0.001	0.0009
Zn	0.02	0.015	0.01	0.01
Mg	0.9	0.4	0.2	0.1
As	0.015	0.008	0.003	0.001
S	300	120	50	20
K	500	200	80	35
Cr	0.0025	0.004	0.004	0.003
Cu	1.5	0.5	0.2	0.1
Hg	0.0005	0.0002	6E-05	2E-05
Cd	0.0002	5E-05	5E-05	2.5E-05
P	0.25	0.13	0.06	0.04
Na	2000	700	300	80
Ni	0.04	0.01	0.003	0.001
Cl	3000	1000	300	40
Pb	0.0025	0.002	0.002	0.002
Al	40	50	60	50

Add time period

Stored ecotoxicity, based on the “Substance transfer – default” template:

Material transfer

Stored ecotoxicity

Substance transfer - default

Define transfer coefficient (applied to all material fractions)

Add material property | Add output column | Add compartment

Material property	soil - stored (%)	water - stored (%)	Degradation (%)
Ca	50	50	0
Cl	50	50	0
F	50	50	0
H	50	50	0
K	50	50	0
N	50	50	0
Na	50	50	0
O	50	50	0
P	50	50	0
S	50	50	0
Ag	50	50	0
Al	50	50	0
As	50	50	0
B	50	50	0
Ba	50	50	0
Be	50	50	0
Br	50	50	0
Cd	50	50	0
Co	50	50	0
Cr	50	50	0
Cu	50	50	0
Fe	50	50	0
Hg	50	50	0
Mg	50	50	0
Mn	50	50	0
Mo	50	50	0
Ni	50	50	0
Pb	50	50	0
Sb	50	50	0
Se	50	50	0
Mo	50	50	0
Ni	50	50	0
Pb	50	50	0
Sb	50	50	0
Se	50	50	0
Sn	50	50	0
Sr	50	50	0
Ti	50	50	0
V	50	50	0
Zn	50	50	0

Leachate collection, based on the “Mass transfer over years” template:

Material transfer

Leachate collection

Mass transfer over years

Time period duration (years)

Time period duratic	Collected %	Not collected %
10	97	3
35	90	10
55	80	20

Add output column

Waste water treatment plant, based on the “substance transfer – default” template:

Material transfer

WWTP - leachate

Substance transfer - default

Define transfer coefficient (applied to all material fractions)

Add material property | Add output column | Add compartment

Material property	water - surface wat	Degradation (%)
Ca	15	85
Cl	15	85
K	15	85
Na	15	85
P	15	85
S	15	85
Al	15	85
As	30	70
Cd	15	85
Cr	70	30
Cu	50	50
Fe	15	85
Hg	15	85
Mg	15	85
Mn	15	85
Mo	15	85
Ni	15	85
Pb	15	85
Sb	15	85
Sn	15	85
Zn	30	70

Process exchanges

WWTP - leachate

External processes

Add external process

Name	Amount	Unit	Per	Comment
View Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DK, kWh, 2006	0.004	kWh	kg Total Wet Weight	

Elementary exchanges

Add elementary exchange

Emissions to groundwater, based on the "substance transfer – default" template:

Material transfer

Emitted to groundwater

Substance transfer - default

Define transfer coefficient (applied to all material fractions)

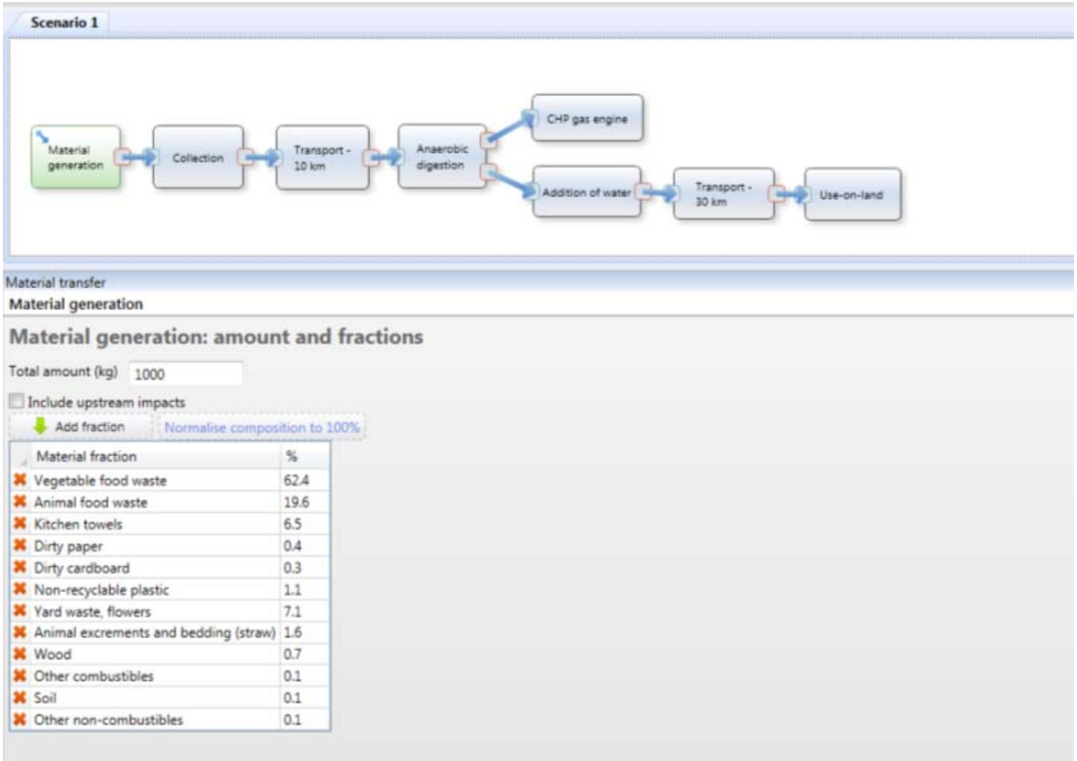
Add material property | Add output column | Add compartment

Material property	water - ground- (%)	Degradation (%)
Ca	100	0
Cl	100	0
F	100	0
H	100	0
K	100	0
N	100	0
Na	100	0
O	100	0
P	100	0
S	100	0
Ag	100	0
Al	100	0
As	100	0
B	100	0
Ba	100	0
Be	100	0
Br	100	0
Cd	100	0
Co	100	0
Cr	100	0
Cu	100	0
Fe	100	0
Hg	100	0
Mg	100	0
Mn	100	0
Mo	100	0
Ni	100	0

Mo	100	0
Ni	100	0
Pb	100	0
Sb	100	0
Se	100	0
Sn	100	0
Sr	100	0
Ti	100	0
V	100	0
Zn	100	0

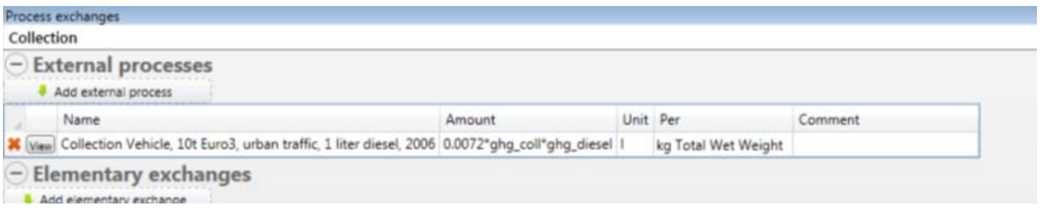
1.2 Anaerobic digestion (AD) scenario

Material generation, based on "Material generation" template:



Material fraction	%
Vegetable food waste	62.4
Animal food waste	19.6
Kitchen towels	6.5
Dirty paper	0.4
Dirty cardboard	0.3
Non-recyclable plastic	1.1
Yard waste, flowers	7.1
Animal excrements and bedding (straw)	1.6
Wood	0.7
Other combustibles	0.1
Soil	0.1
Other non-combustibles	0.1

Collection, based on the "basic process" template:

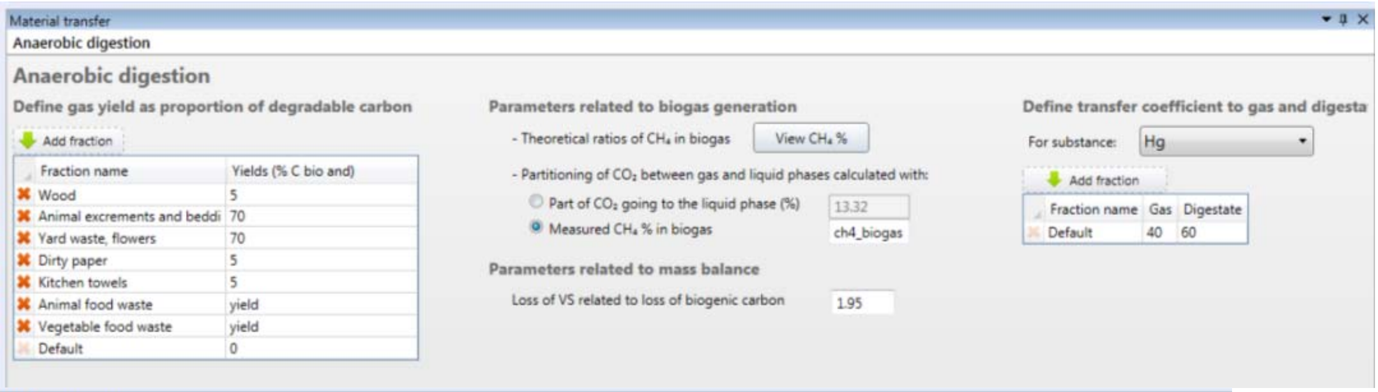


Name	Amount	Unit	Per	Comment
Collection Vehicle, 10t Euro3, urban traffic, 1 liter diesel, 2006	0.0072*ghg_coll*ghg_diesel	l	kg Total Wet Weight	

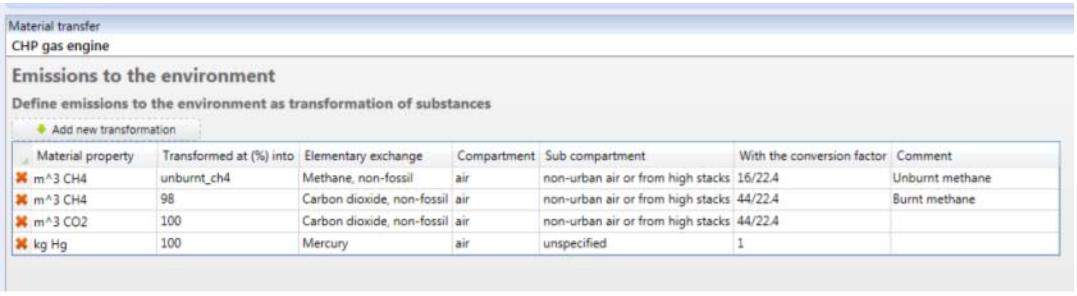
Transport, based on the "basic process" template:

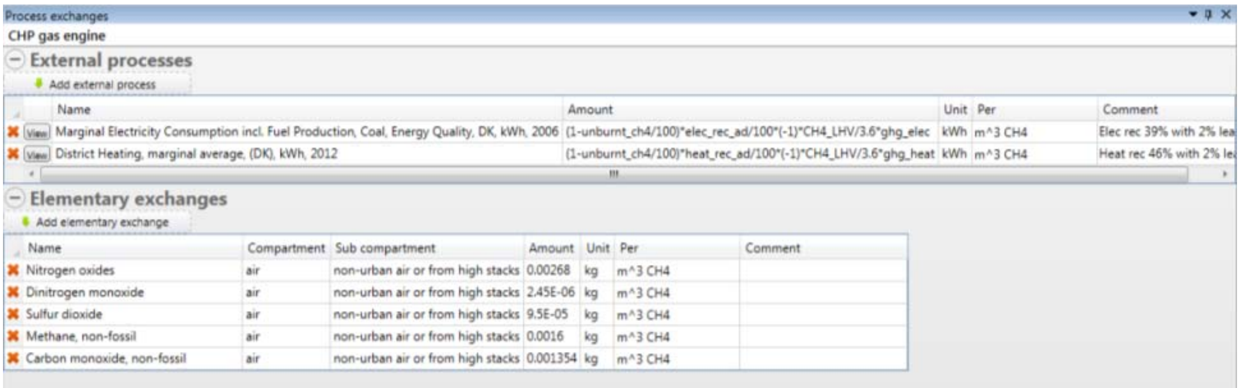
Name	Amount	Unit	Per	Comment
Collection Vehicle, 10t Euro3, urban traffic, 1 liter diesel, 2006	10*0.00009*ghg_diesel	l	kg Total Wet Weight	change the 1 by the number c

Anaerobic digestion, based on the "Anaerobic digestion" template:

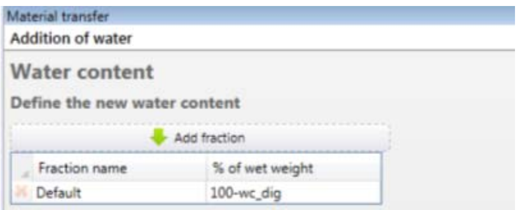


CHP gas engine, based on "Emissions to the environment" template:

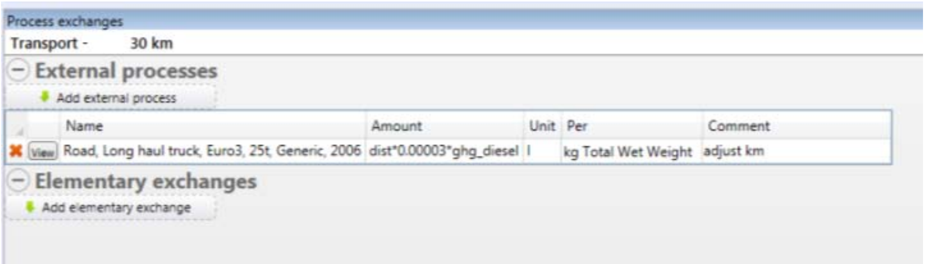




Addition of water, based on the "Water content" template:



Transport of digestate, based on the "Basic process" template:



Process exchanges

Transport - 30 km

External processes

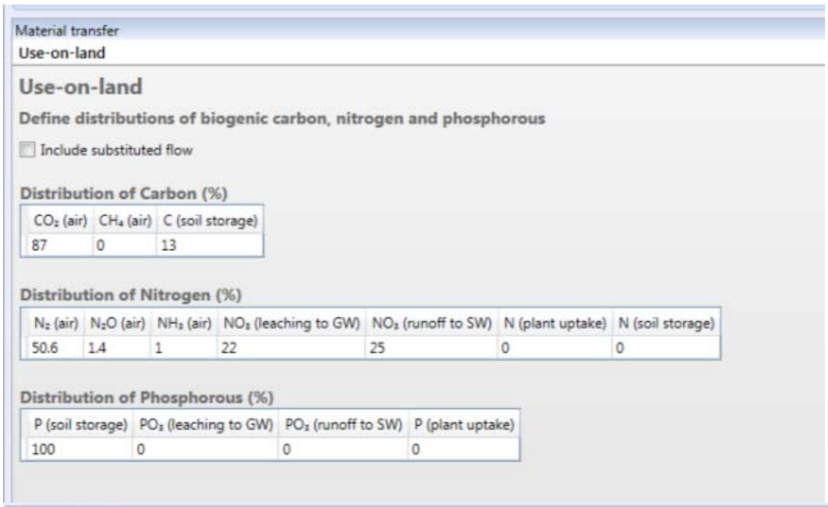
Add external process

Name	Amount	Unit	Per	Comment
Road, Long haul truck, Euro3, 25t, Generic, 2006	dist*0.00003*ghg_diesel	l	kg Total Wet Weight	adjust km

Elementary exchanges

Add elementary exchange

Use on land, based on the “Use on land” template:



Material transfer

Use-on-land

Use-on-land

Define distributions of biogenic carbon, nitrogen and phosphorous

Include substituted flow

Distribution of Carbon (%)

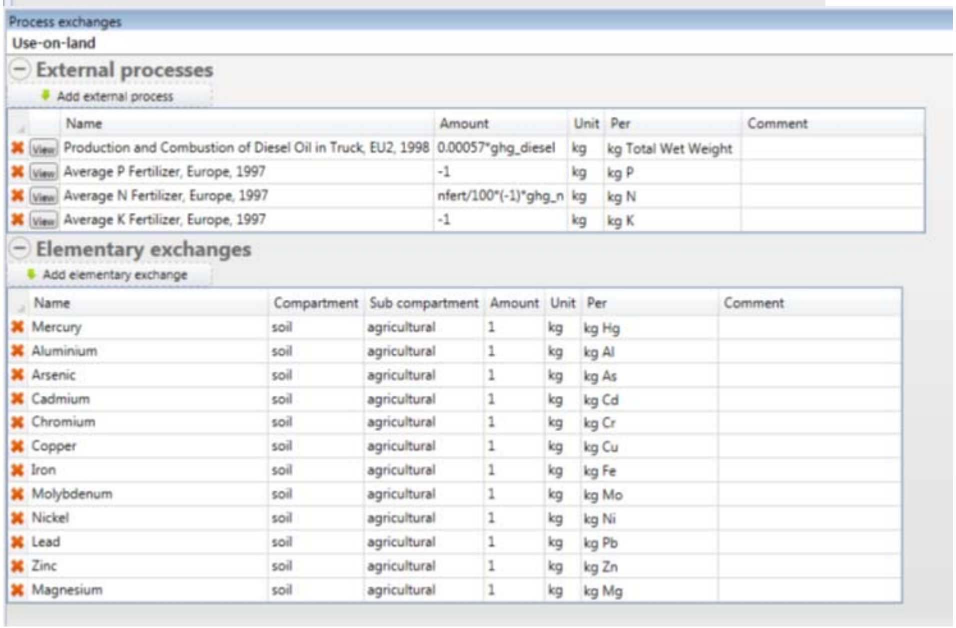
CO_2 (air)	CH_4 (air)	C (soil storage)
87	0	13

Distribution of Nitrogen (%)

N_2 (air)	N_2O (air)	NH_3 (air)	NO_3 (leaching to GW)	NO_3 (runoff to SW)	N (plant uptake)	N (soil storage)
50.6	1.4	1	22	25	0	0

Distribution of Phosphorous (%)

P (soil storage)	PO_3 (leaching to GW)	PO_3 (runoff to SW)	P (plant uptake)
100	0	0	0



Process exchanges

Use-on-land

External processes

Add external process

Name	Amount	Unit	Per	Comment
Production and Combustion of Diesel Oil in Truck, EU2, 1998	0.00057*ghg_diesel	kg	kg Total Wet Weight	
Average P Fertilizer, Europe, 1997	-1	kg	kg P	
Average N Fertilizer, Europe, 1997	nfert/100*(-1)*ghg_n	kg	kg N	
Average K Fertilizer, Europe, 1997	-1	kg	kg K	

Elementary exchanges

Add elementary exchange

Name	Compartment	Sub compartment	Amount	Unit	Per	Comment
Mercury	soil	agricultural	1	kg	kg Hg	
Aluminium	soil	agricultural	1	kg	kg Al	
Arsenic	soil	agricultural	1	kg	kg As	
Cadmium	soil	agricultural	1	kg	kg Cd	
Chromium	soil	agricultural	1	kg	kg Cr	
Copper	soil	agricultural	1	kg	kg Cu	
Iron	soil	agricultural	1	kg	kg Fe	
Molybdenum	soil	agricultural	1	kg	kg Mo	
Nickel	soil	agricultural	1	kg	kg Ni	
Lead	soil	agricultural	1	kg	kg Pb	
Zinc	soil	agricultural	1	kg	kg Zn	
Magnesium	soil	agricultural	1	kg	kg Mg	

2 LCIA methods used

Table S2: Environmental impact categories and normalization references of the ILCD recommended methods. References given are first to method, next to normalization references.

Impact category	Method	Unit	Normalisation factor	Year and space of normalisation, reference, remark
Climate change	IPCC (Forster et al., 2007)	kg CO_2-Eq	7730	Laurent et al., 2011a
Ozone depletion	EDIP97 (WMO) (Wenzel et al., 1997)	kg CFC-11-Eq	2.05E-2	Laurent et al., 2011a
Human toxicity, cancer effects	USEtox (Rosenbaum et al., 2008)	CTUh	3.25E-5	Laurent et al., 2011b
Human toxicity, non-cancer effects	USEtox (Rosenbaum et al., 2008)	CTUh	8.14E-4	Laurent et al., 2011b
Particulate matter/ respiratory inorganics	Updated from Humbert (2009), from SI of Laurent et al. (2012)	kg $PM_{2.5}$-eq	4.71	From SI of Laurent et al. (2012)
Acidification	ReCiPe (Van Zelm et al., 2008)	kg SO_2-Eq	49.9	Sleeswijk et al., 2008
Eutrophication, terrestrial	CML (Guinée et al. 2002)	kg NOx-Eq	356	Huijbregts et al, 2003 and CML(2012) [3]
Photochemical ozone formation	ReCiPe (Van Zelm et al., 2008)	kg NMVOC	52.9	Sleeswijk et al., 2008
Eutrophication, freshwater	ReCiPe (Van Zelm et al., 2008)	kg P-Eq	0.69	Sleeswijk et al., 2008
Ecotoxicity (freshwater)	USEtox (Rosenbaum et al., 2008)	CTUe	5060	Laurent et al., 2011b
Resource depletion, mineral and fossil	CML(Guinée et al., 2002)	kg antimony-Eq	0.95	Guinée et al., 2002 [1]

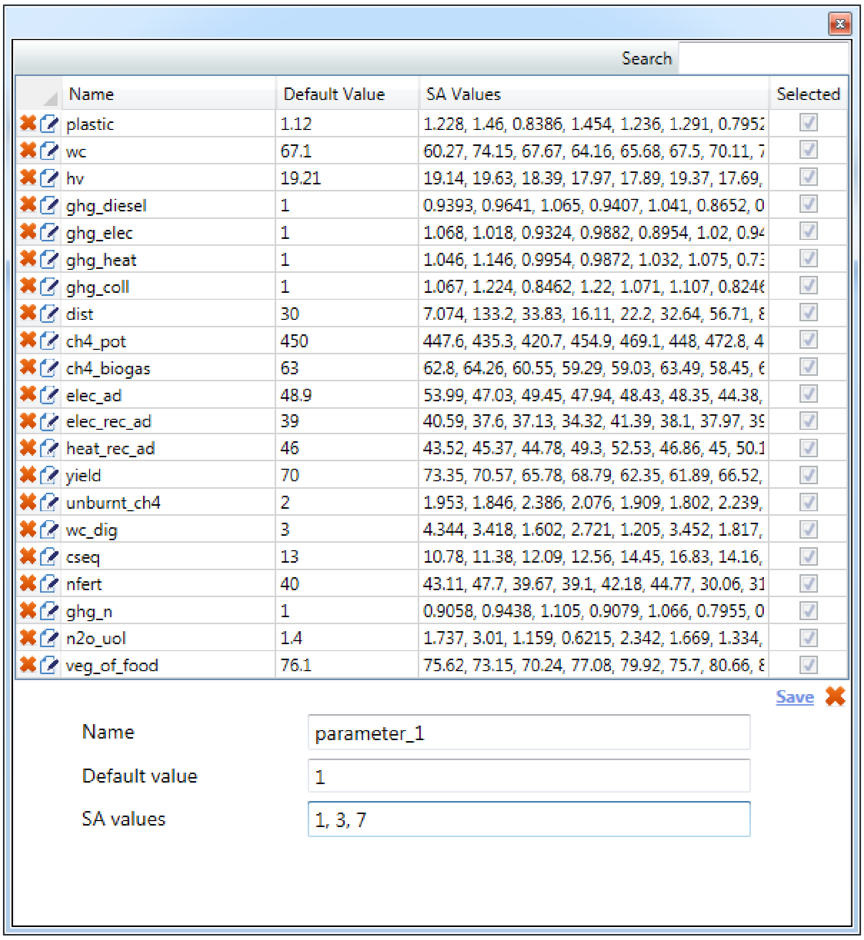
[1]Calculated based on population in EU-15 1995 assumed to: 380 million, and the total value for 1995: 1.4E+11 kg PO43- eq. / yr

3 Uncertainty propagation

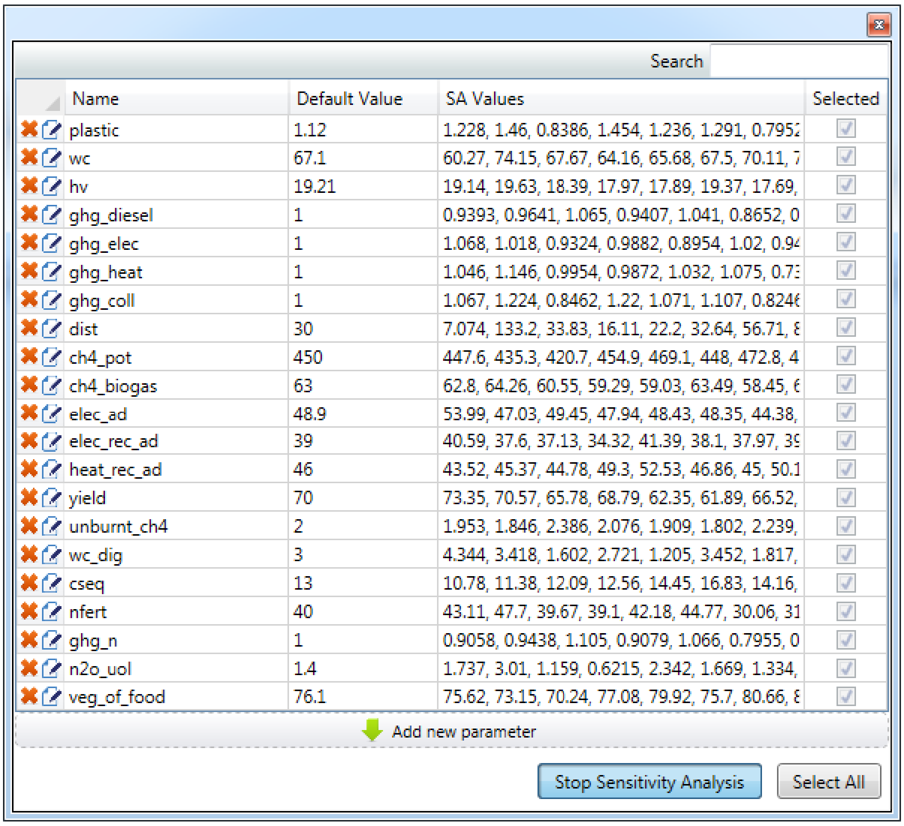
In this section we present briefly how uncertainty data is input in EASETECH, how systems are parameterized and how results are displayed.

3.1 The table of parameters

Parameters are added simply by specifying a name to the parameter, a default value and a list of values to be used when running calculations in “sensitivity analysis” mode.

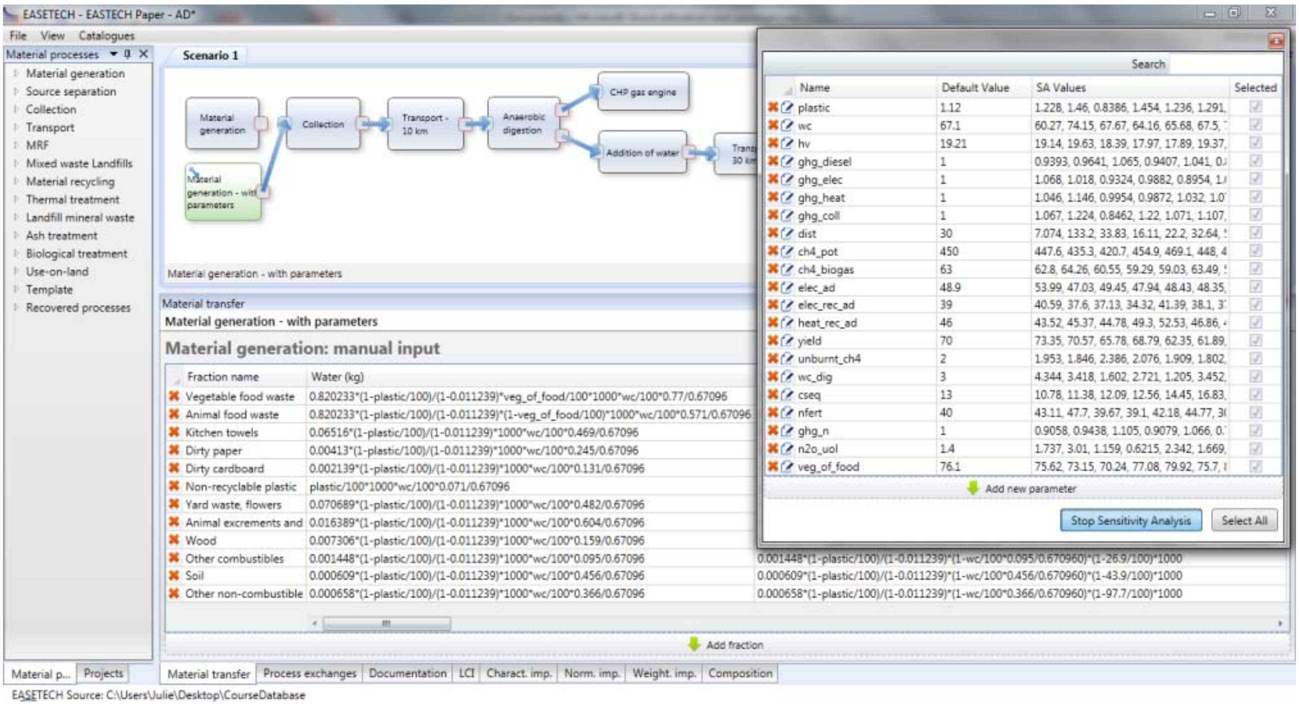


To run the calculations in "sensitivity analysis" mode, at least one parameter has to be selected and then the user should click on the "Run Sensitivity analysis" button.



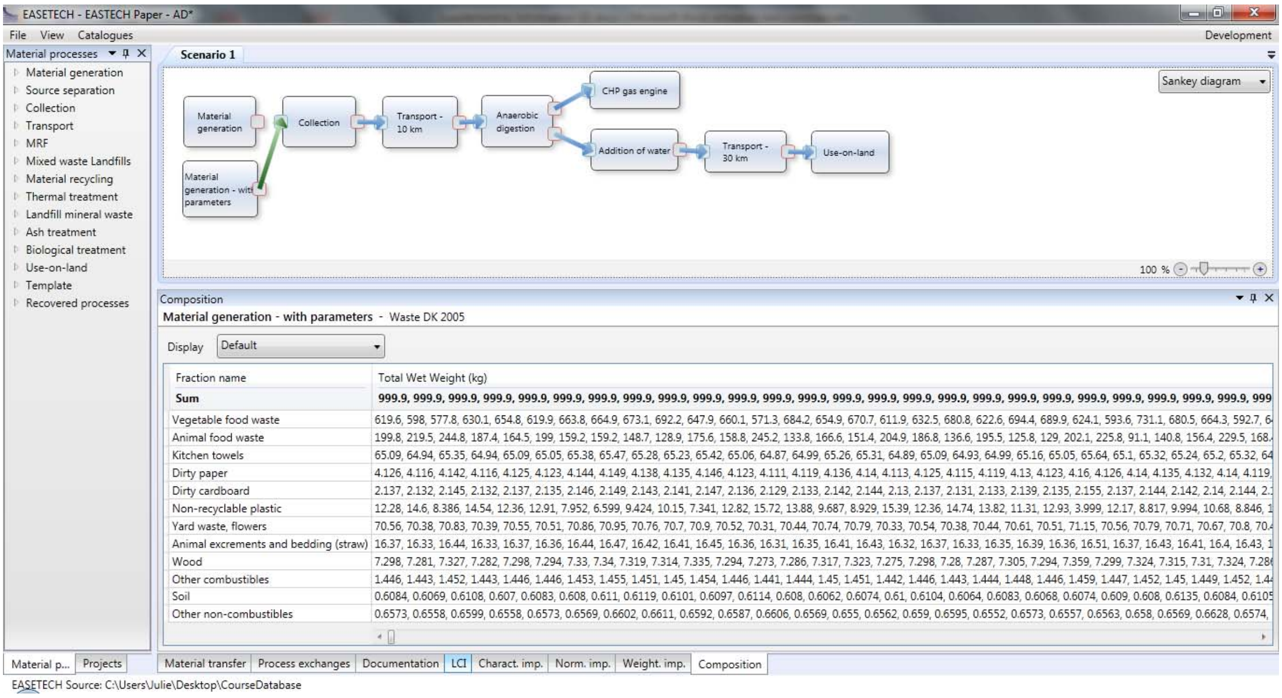
3.2 Material generation

The following figure is a screenshot showing how the waste generation was parameterised using four parameters: the content of plastic in the waste (“plastic”), the water content of the whole waste (“wc”), the lower heating value (“hv”) and the methane potential (“ch4_pot”). It can be observed that to parameterize material generation, we use a different process than the classical one (presented in section Part II, Section 1.3). This process allows free definition of amounts of different properties. The screenshot presents the formulas used for the water content in the 12 material fractions. The pop-up window on the right side shows the table of parameters where all parameters are defined, together with their default value and the list of numbers to be tested. Here each parameter has a list of 1000 values randomly sampled in the distributions defined earlier. This lists of random values were obtained using a small excel macro.



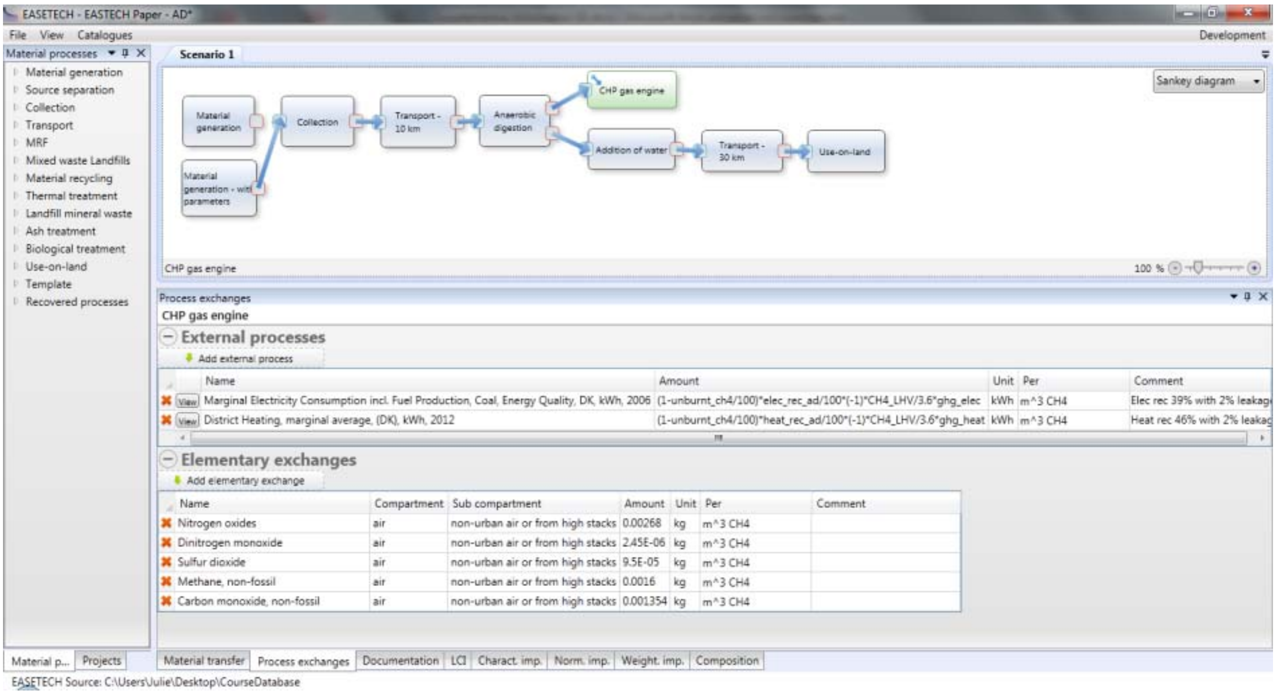
3.3 Material composition calculation

The output of this process can be computed and is presented in the next figure. It can be observed that each result field shows the 1000 values obtained as a result of the computation with 1000 values for each parameter. All table results can always be copied and pasted into Excel, which offers simple tools to convert a cell of 1000 values into 1000 cells that can be easily analysed.

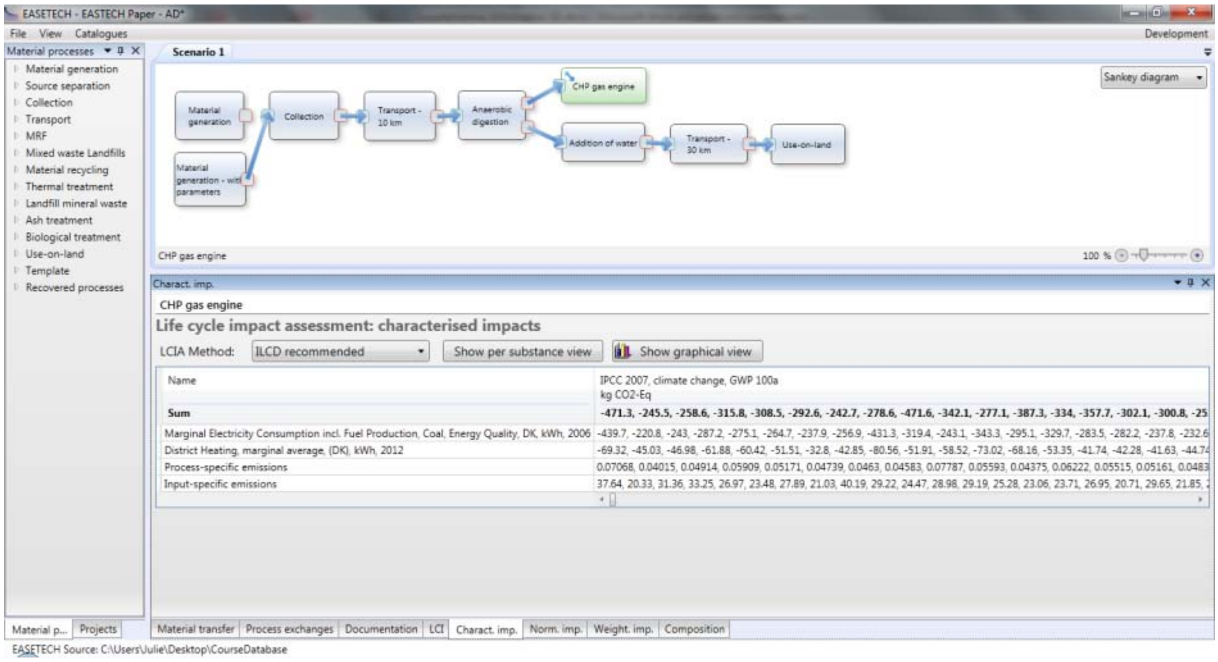


3.4 LCI data in material process

In the same way, data of the other processes have been parameterized. Below is presented the example for the “CHP gas engine” material process.



3.5 Calculation of the characterised impact



NB: the display of the results will be improved in the future, but it is still possible to make full use of the results by using excel tools.

4 References

Clavreul, J., Guyonnet, D., Christensen, T.H., 2012. Quantifying uncertainty in LCA-modelling of waste management systems. Waste Management 32, 2482–2495.

CML (2012). CML-IA Characterisation Factors. Excel spreadsheet [Online] http://www.leidenuniv.nl/cml/ssp/databases/cmlia/cmlia.zip, Accessed 31 January 2013

Forster, P., Ramaswamy, V., Artaxo, P., Berntsen, T., Betts, R., Fahey, D.W., Haywood, J., Lean, J., Lowe, D.C., Myhre, G., Nganga, J., Prinn, R., Raga, G., Schulz, M., Van Dorland, R., 2007. Changes in atmospheric constituents and in radiative forcing. In: Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K.B., Tignor, M., Miller, H.L. (Eds.), Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

Guinée, J.B., Gorrée, M., Heijungs, R., Huppes, G., Kleijn, R., Koning, A. de, Oers, L. van, Wegener Sleeswijk, A., Suh, S., Udo de Haes, H.A., Bruijn, H. de, Duin, R. van, Huijbregts, M.A.J., 2002. Handbook on life cycle assessment. Operational guide to the ISO standards. I: LCA in perspective. IIa: Guide. IIb: Operational annex. III: Scientific background. Kluwer Academic Publishers, ISBN 1-4020-0228-9, Dordrecht, 692 pp.

Huijbregts, M.a.J., Breedveld, L., Huppes, G., de Koning, A., van Oers, L., Suh, S. (2003) Normalisation figures for environmental life-cycle assessment. Journal of Cleaner Production 11, 737–748.

Humbert S., 2009. Geographically differentiated life-cycle impact assessment of human health. Ph.D. Dissertation, AAT 3402614, University of California, CA, USA.

Laurent, A., Olsen, S. I., Hauschild, M. Z., 2011a. Normalization in EDIP97 and EDIP2003: updated European inventory for 2004 and guidance towards a consistent use in practice. International Journal of Life Cycle Assessment 16, 401–409.

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