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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 CO₂ 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 CO₂ into the air.

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

---

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

![Example of a FitNesse Wiki page testing the conceptual model](image-url)
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):

<table>
<thead>
<tr>
<th>Category</th>
<th>Fractile name</th>
<th>Weight (%)</th>
<th>V (%)</th>
<th>Ash (%)</th>
<th>C (%)</th>
<th>Energy (MJ/kg)</th>
<th>C bio (%)</th>
<th>C bio and (%)</th>
<th>C fossil (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Organics</strong></td>
<td>Vegetable food waste</td>
<td>79.09</td>
<td>23</td>
<td>18.8</td>
<td>3.2</td>
<td>13.7</td>
<td>4.3</td>
<td>40.3</td>
<td>0.038</td>
</tr>
<tr>
<td><strong>Organics</strong></td>
<td>Animal food waste</td>
<td>57.14</td>
<td>42.9</td>
<td>31.2</td>
<td>8.7</td>
<td>136.5</td>
<td>95.4</td>
<td>12.9</td>
<td>0.263</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Newspapers</td>
<td>12.95</td>
<td>87</td>
<td>91.6</td>
<td>8.2</td>
<td>17.07</td>
<td>24.6</td>
<td>7.3</td>
<td>0.024</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Magazines</td>
<td>6.2</td>
<td>93.8</td>
<td>95.6</td>
<td>3.4</td>
<td>11.47</td>
<td>8.6</td>
<td>8.6</td>
<td>0.021</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Newspapers</td>
<td>12.95</td>
<td>87</td>
<td>91.6</td>
<td>8.2</td>
<td>17.07</td>
<td>24.6</td>
<td>7.3</td>
<td>0.024</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Advertisements</td>
<td>8.75</td>
<td>91.3</td>
<td>72.6</td>
<td>27.4</td>
<td>13.05</td>
<td>34.3</td>
<td>12.9</td>
<td>0.173</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Books, phone books</td>
<td>4.0</td>
<td>91.3</td>
<td>93.2</td>
<td>17.8</td>
<td>13.03</td>
<td>40.4</td>
<td>21.4</td>
<td>0.163</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Office paper</td>
<td>8.75</td>
<td>91.3</td>
<td>79.3</td>
<td>22.8</td>
<td>12.53</td>
<td>27.3</td>
<td>20.6</td>
<td>0.188</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Other paper</td>
<td>7.27</td>
<td>90.8</td>
<td>82.8</td>
<td>17.2</td>
<td>13.91</td>
<td>28.1</td>
<td>21.9</td>
<td>0.192</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Paper and carton containers</td>
<td>22.25</td>
<td>77.7</td>
<td>85.6</td>
<td>13.4</td>
<td>14.97</td>
<td>40.9</td>
<td>13.1</td>
<td>0.294</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Other cardboard</td>
<td>16.52</td>
<td>83.9</td>
<td>84</td>
<td>14</td>
<td>15.08</td>
<td>40.7</td>
<td>13.2</td>
<td>0.265</td>
</tr>
<tr>
<td><strong>Composite</strong></td>
<td>Composites</td>
<td>16.54</td>
<td>84.2</td>
<td>98.8</td>
<td>1.2</td>
<td>2.023</td>
<td>40</td>
<td>13.5</td>
<td>0.266</td>
</tr>
<tr>
<td><strong>Composite</strong></td>
<td>Composite</td>
<td>16.54</td>
<td>84.2</td>
<td>98.8</td>
<td>1.2</td>
<td>2.023</td>
<td>40</td>
<td>13.5</td>
<td>0.266</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Other paper</td>
<td>7.27</td>
<td>90.8</td>
<td>82.8</td>
<td>17.2</td>
<td>13.91</td>
<td>28.1</td>
<td>21.9</td>
<td>0.192</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Kitchen towels</td>
<td>48.86</td>
<td>93.5</td>
<td>97.3</td>
<td>2.7</td>
<td>18.97</td>
<td>44.7</td>
<td>25.2</td>
<td>0.042</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Dry paper</td>
<td>24.47</td>
<td>73.8</td>
<td>91.1</td>
<td>8.8</td>
<td>16.17</td>
<td>44.6</td>
<td>13</td>
<td>0.035</td>
</tr>
<tr>
<td><strong>Fiber</strong></td>
<td>Dirty outdoors</td>
<td>13.1</td>
<td>99.3</td>
<td>95.1</td>
<td>4.9</td>
<td>14.97</td>
<td>42.7</td>
<td>14.2</td>
<td>0.411</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Soft plastic</td>
<td>14.31</td>
<td>85.9</td>
<td>95.4</td>
<td>4.6</td>
<td>40.05</td>
<td>6.0</td>
<td>6.0</td>
<td>0.001</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Plastic bottles</td>
<td>10.46</td>
<td>89.3</td>
<td>95.9</td>
<td>6.2</td>
<td>36.04</td>
<td>0.006</td>
<td>0</td>
<td>76.8</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Paint</td>
<td>3.29</td>
<td>94.9</td>
<td>97.8</td>
<td>2.2</td>
<td>37.41</td>
<td>0.4</td>
<td>0</td>
<td>79.3</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Paint</td>
<td>3.29</td>
<td>94.9</td>
<td>97.8</td>
<td>2.2</td>
<td>37.41</td>
<td>0.4</td>
<td>0</td>
<td>79.3</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Non-recyclable plastic</td>
<td>7.12</td>
<td>92.9</td>
<td>94.5</td>
<td>5.5</td>
<td>31.96</td>
<td>0.355</td>
<td>0</td>
<td>76.8</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Organics</td>
<td>48.21</td>
<td>91.8</td>
<td>76</td>
<td>24</td>
<td>13.95</td>
<td>42.1</td>
<td>7.2</td>
<td>0.068</td>
</tr>
<tr>
<td><strong>Plastic</strong></td>
<td>Composite</td>
<td>16.54</td>
<td>84.2</td>
<td>98.8</td>
<td>1.2</td>
<td>2.023</td>
<td>40</td>
<td>13.5</td>
<td>0.266</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Other paper</td>
<td>7.27</td>
<td>90.8</td>
<td>82.8</td>
<td>17.2</td>
<td>13.91</td>
<td>28.1</td>
<td>21.9</td>
<td>0.192</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Other paper</td>
<td>7.27</td>
<td>90.8</td>
<td>82.8</td>
<td>17.2</td>
<td>13.91</td>
<td>28.1</td>
<td>21.9</td>
<td>0.192</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>Other paper</td>
<td>7.27</td>
<td>90.8</td>
<td>82.8</td>
<td>17.2</td>
<td>13.91</td>
<td>28.1</td>
<td>21.9</td>
<td>0.192</td>
</tr>
</tbody>
</table>

### Material transfer

- **Material transfer**
- **Process exchanges**
- **Documentation**
- **IT**
- **Character imp**
- **Item imp.**
- **Weight imp.**
- **Composition**
“Elementary exchanges” catalogue (4b):

<table>
<thead>
<tr>
<th>Compartiment</th>
<th>Sub-compartment</th>
<th>Name</th>
<th>Unit</th>
<th>Formula</th>
<th>CashNumber</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td>Carbon-monoxide, from soil or biomass stock</td>
<td>kg</td>
<td>C3H4O</td>
<td>000003-80-0</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Methane, from soil or biomass stock</td>
<td>kg</td>
<td>C2H6</td>
<td>000007-42-4</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 3.5 Baseline</td>
<td>kg</td>
<td>C4H10D2</td>
<td>000113-43-4</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 1 Permanente</td>
<td>kg</td>
<td>C4H10D</td>
<td>000017-43-0</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 1 Pescatore</td>
<td>kg</td>
<td>CH3D</td>
<td>000013-42-1</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Enrangepass</td>
<td>kg</td>
<td>CH4N2D</td>
<td>000248-11-3</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Montreal</td>
<td>kg</td>
<td>CH4N2D2</td>
<td>000026-14-0</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 3 Methylin</td>
<td>kg</td>
<td>CH4N2</td>
<td>000007-85-3</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 3 Methylin 3</td>
<td>kg</td>
<td>CH4N3</td>
<td>000011-95-9</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Micronew acid</td>
<td>kg</td>
<td>C8H8N2D6</td>
<td>000893-10-6</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Propyl</td>
<td>kg</td>
<td>CH3CH2O</td>
<td>000007-65-0</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Methyl-3 Butanol</td>
<td>kg</td>
<td>CH3CH2CHOCH3</td>
<td>000012-10-1</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Methyl-3 Butanol</td>
<td>kg</td>
<td>CH3CH2CHOCH3</td>
<td>000012-10-1</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Acetophenone</td>
<td>kg</td>
<td>C8H8O2</td>
<td>000007-30-9</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>Low population density, long-term: 2 Acetophenone</td>
<td>kg</td>
<td>C8H8O2</td>
<td>000007-30-9</td>
</tr>
</tbody>
</table>

“Impact categories” catalogue (4c):

<table>
<thead>
<tr>
<th>Impact category</th>
<th>Characterisation Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline climate change, GWP 100y</td>
<td>1</td>
</tr>
<tr>
<td>Non-refractive air or from high</td>
<td>1</td>
</tr>
<tr>
<td>Carbon dioxide, from solid</td>
<td>1</td>
</tr>
<tr>
<td>Low population density, low</td>
<td>1</td>
</tr>
<tr>
<td>Carbon dioxide, from solid</td>
<td>1</td>
</tr>
<tr>
<td>Lower stratosphere = upper</td>
<td>1.571</td>
</tr>
<tr>
<td>Carbon dioxide, from solid</td>
<td>1.571</td>
</tr>
<tr>
<td>Lower stratosphere = upper</td>
<td>1.571</td>
</tr>
<tr>
<td>Carbon dioxide, from solid</td>
<td>1.571</td>
</tr>
<tr>
<td>Material transfer from</td>
<td>1</td>
</tr>
<tr>
<td>Non-refractive air or from high</td>
<td>1</td>
</tr>
<tr>
<td>Material transfer from</td>
<td>1</td>
</tr>
<tr>
<td>Lower stratosphere = upper</td>
<td>1</td>
</tr>
<tr>
<td>Material transfer from</td>
<td>1</td>
</tr>
<tr>
<td>Non-refractive air or from high</td>
<td>1</td>
</tr>
<tr>
<td>Material transfer from</td>
<td>1</td>
</tr>
</tbody>
</table>
“Methods” catalogue (4d):

```
![Image of the "Methods" catalogue]
```

“Interfaces” catalogue (4e):

```
![Image of the "Interfaces" catalogue]
```
“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) = \( \text{water} \% \text{fraction} \times \frac{\text{TotalAmount}}{100} \times \frac{\text{percent}}{100} \times \frac{\text{TotalAmount}}{100} \)
- vs(kg) = \( \text{VS} \% \text{fraction} \times \frac{\text{TotalAmount}}{100} \times \frac{\text{percent}}{100} \)
- ash(kg) = \( \text{ash} \% \text{fraction} \times \frac{\text{TotalAmount}}{100} \times \frac{\text{percent}}{100} \)
- energy (MJ) = \( \text{energy} \% \text{fraction} \times \frac{\text{TS} \% \text{fraction}}{100} \times \frac{\text{percent}}{100} \times \frac{\text{TotalAmount}}{100} \)
- for all other material properties: materialproperty(kg) = \( \text{materialproperty} \% \text{fraction} \times \frac{\text{TS} \% \text{fraction}}{100} \times \frac{\text{percent}}{100} \times \frac{\text{TotalAmount}}{100} \)

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.
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

**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

![Image of material composition](image.png)

**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,

\[
\text{outputNumber.fraction.property} = \text{input.fraction.property} \times \frac{\text{TC(property, fraction, outputNumber)}}{100}
\]

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**

<table>
<thead>
<tr>
<th>Fraction name</th>
<th>Total Wet Weight (kg)</th>
<th>TS (kg)</th>
<th>Water (kg)</th>
<th>VS (kg)</th>
<th>Ash (kg)</th>
<th>Ener gy (MJ)</th>
<th>C bio (kg)</th>
<th>C bio and (kg)</th>
<th>Ca (kg)</th>
<th>Cl (kg)</th>
<th>F (kg)</th>
<th>H (kg)</th>
<th>K (kg)</th>
<th>N (kg)</th>
<th>Na (kg)</th>
<th>O (kg)</th>
<th>P (kg)</th>
<th>S (kg)</th>
<th>Ag (kg)</th>
<th>Al (kg)</th>
<th>As (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vegetable food waste</td>
<td>21</td>
<td>4.8</td>
<td>16</td>
<td>4.5</td>
<td>0.2</td>
<td>88.38</td>
<td>2.2</td>
<td>94</td>
<td>0.01</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3</td>
<td>0.0</td>
<td>1.9</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.2</td>
</tr>
<tr>
<td>Office paper</td>
<td>9.005</td>
<td>0.2</td>
<td>785</td>
<td>6.5</td>
<td>1.7</td>
<td>103</td>
<td>3.0</td>
<td>65</td>
<td>1.693</td>
<td>0.01</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.7</td>
</tr>
</tbody>
</table>

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**

Output 1 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: $9.66 \times 8 \times 98/100 = 9.47 \text{ E-8 kg}$

- all others equal to the fraction “vegetable food waste” in the input
- for fraction “office paper”:
  - VS: $6.516 \times 97/100 = 6.321 \text{ kg}$
  - Hg: $2.925 \times 90/100 = 2.632 \times 7 \text{ kg}$

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,

$$\text{outputNumber.fraction.property} = \text{input.fraction.property} \times \text{TC(property, outputNumber)/100}$$

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.
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.

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,

\[
\text{outputNumber.fraction.property} = \text{input.fraction.property} \times \text{TC(fraction, outputNumber)}/100
\]

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 columnns.
- 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.
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”.

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,

\[
\text{output.fraction.energycontent (MJ)} = \text{input.fraction.energycontent(MJ)} + \sum \text{ForAllProperties [value(fraction, slectedProperty)\times input.fraction.selectedProperty]}
\]

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.
So the calculation of the energy content is:

- for vegetable food waste, energy content (kg) = energy content (kg) + (-2)*water (kg) + (-0.1)*ash (kg) = 88.389 + (-2)*16.17 + (-6)*0.2512 = 54.54 MJ

- for office paper, energy content (kg) = energy content (kg) + (-3)*water (kg) + (-0.1)*ash (kg) = 103 + (-3)*0.7875 + (-6)*1.701 = 90.43 MJ

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,

\[
\text{output.fraction.water (kg)} = \frac{\text{input.fraction.TS (kg)} \times (\text{percent(fraction)})}{(100-\text{percent(fraction))}}
\]

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.
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

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”:
  \[
  \text{output.fraction.selectedMaterialProperty} = \text{input.fraction.selectedMaterialProperty} + \frac{\text{amount(selectedMaterialProperty)} \times \text{input.fraction.TotalWetWeight}}{10^6}
  \]

- if “gas”:
  \[
  \text{output.fraction.selectedMaterialProperty} = \text{input.fraction.selectedMaterialProperty} + \frac{\text{amount(selectedMaterialProperty)} \times (\text{input.fraction.ch4} + \text{input.fraction.co2})}{10^3}
  \]

- if “liquid”:
  \[
  \text{output.fraction.selectedMaterialProperty} = \text{input.fraction.selectedMaterialProperty} + \frac{\text{amount(selectedMaterialProperty)} \times \text{input.fraction.WaterContent}}{10^6}
  \]

- if “energy”:
  \[
  \text{output.fraction.selectedMaterialProperty} = \text{input.fraction.selectedMaterialProperty} + \frac{\text{amount(selectedMaterialProperty)} \times \text{input.fraction.EnergyContent}}{10^3}
  \]

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”.

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If we select “solid”:

![Figure S16: Material transfer of “Addition of substance” in the case of “solid” selection](image1)

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 = 2.925E-7 kg + 1.801E-7 kg = 4.726E-7 kg.

If we select “gas”:

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](image2)

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

![Figure S18: Material composition of the output of the AD process (input of “addition of substance”)](image3)

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:

\[
\text{Ch4\_biogas} = \frac{1}{2} + \frac{168 \times H - 21 \times O - 36 \times N}{112 \times \text{Cbioand}}
\]

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: \[ \text{Sum for all material fractions of } [C_{\text{bio and}} \times \exp(-k \times (n-1)) \times (1-\exp(-k)) \times (1-CH4_{\text{biogas}})] \times 22.4/12 \]
- All other properties are zero, including water, VS and ash.

➢ **Calculation of the Residues output**

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: \[ \text{input.c_bio} - \text{input.c_bio_and} \times (1-\exp(-\text{number_of_years} \times k)) \]
- C bio and is: \[ \text{input.c_bio_and} \times \exp(-\text{number_or_years} \times k) \]
- VS is: \[ \text{input.vs} - \text{vs}_{\text{cbio}} \times \text{input.c_bio_and} \times (1-\exp(-\text{number_or_years} \times k)) \]
- LHV dry [MJ]: \[ \frac{\text{input.lhvdry}}{\text{input.vs}} \times (\text{input.vs} - \text{vs}_{\text{cbio}} \times \text{input.c_bio_and} \times \exp(-\text{number_or_years} \times k)) \]
- All other properties are equal to the input.

➢ **Example:**

![Figure S19: Material transfer of the “Landfill gas generation” process](image)

Gas output, at year n:

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

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).
The input from the landfill gas generation was:

For “Half collected” output,
- Year 1 (period=1): 0.6971 * 10/100 = 0.06971
- Year 2 (period=1): 0.5425 * 10/100 = 0.05425
- 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 = 0.2172
  - 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:

  \[ \text{leachate.year.water} = \text{input.totalWetWeight} \times \frac{\text{netInfiltration}(P)}{\text{density} \times \text{height} \times 10^3} \]

  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:

  \[ \text{leachate.year.substance} = \text{leachate.year.water} \times \text{concentrate(substance, P’)} \times 10^{-6} \]
  
or if easier:
  \[ \text{leachate.year.substance} = \text{input.totalWetWeight} \times \frac{\text{netInfiltration}(P)}{\text{density} \times \text{height} \times 10^3} \times \text{concentrate(substance, P’)} \times 10^{-6} \]
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:

\[
\text{Input.fraction.substance} - \sum_{\text{for all years}} [\text{leachate.year.water} \times \text{concentrate(substance, P')*10^{-6}} \times \text{input.fraction.substance/input.substance(of_all_fractions)}]
\]

When connecting the process described in Figure

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
- For “Residues” output, all properties are the same as the input except from N and P, let’s 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

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:

\[
\text{Ch}_4\text{biogas} = \frac{1}{2} \times \frac{168 \times H - 21 \times O - 36 \times N}{112 \times \text{Cbioand}}
\]

(1)

(1)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

  \[
  \text{MeasuredCH4}\% = \frac{100 \times \sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \frac{\text{ch4\_biogas}}{100}\right)}{\sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \frac{\text{ch4\_biogas}}{100}\right) + \sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \left(1-\frac{\text{ch4\_biogas}}{100}\right) \times \left(1-\frac{\text{co2\_liq}}{100}\right)\right)}
  \]

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

  Co2liq is calculated like this:

  \[
  \text{Co2liq} = \frac{100 - \left(\text{measured\_ch4}\%\right)}{\text{measured\_ch4}\%} \times \frac{\sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \text{ch4\_biogas}/100\right)}{\sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \left(1-\text{ch4\_biogas}/100\right)\right)}
  \]

- **Calculation of the GAS output**

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

  - C bio [kg] is: \( \sum_{\text{all material fractions}} \left(\frac{\text{yield}}{100} \times \text{C\_bio\_and} \times \left(1-\frac{\text{co2\_liq}}{100}\right) \times \left(1-\text{ch4\_biogas}/100\right)\right) \)
- CH4 [m³] is: Sum_for_all_material_fractions_of \((\text{yield}/100 \times \text{C_bio_and} \times \text{ch4_biogas}/100)\) *22.4/12
- CO2 [m³] is: Sum_for_all_material_fractions_of \((\text{yield}/100 \times \text{C_bio_and} \times (1-\text{ch4_biogas}/100)) \times (1-\text{co2_liq}/100)\) *22.4/12
- Pollutants [kg]: Sum_for_all_material_fractions_of \((\text{pollutant}_\text{kg(fraction)} \times \text{TC_of_pollutants_to_gas}/100)\)
- All other properties are zero, including water, VS, ash, Energy, C bio and.

➤ **Calculation of the DIGESTATE output**

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

➤ **Example:**

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. **With radio button on “Part of CO2…”**

![Figure S26: Material transfer of the “anaerobic digestion” process](image)

The value “Measured CH4% in biogas” is:

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

The gas output is:

- C bio [kg] = 70/100 \times 2.043 \times (1-10/100*(1-54.45/100)) + 10/100 \times 1.693 \times (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 m³
- 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 m³
- N [kg]: 0.09177*30/100 + 0.008217*50/100 = 0.03164 kg

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

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 m³
- 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 m³
- N [kg]: 0.09177*30/100 + 0.008217*50/100 = 0.03164 kg

![Figure S30: Composition of the gas output](image)

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

![Figure S31: Composition of the digestate output](image)

Figure S32 provides explanations about the calculations happening 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 ticked, 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 CO₂-eq/kg).

![Figure S33: Example used in Section 2](image)

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](image)

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.

![Image](SI-35.png)

**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

![Image](SI-36.png)

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

Figure S38 presents the 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:
  - Carbon dioxide: amount(test3UsedInTest2) * amountOfCarbonDioxideInLci(test3) = 2 * 4 = 8.
  - Methane: amount(test3UsedInTest2) * amountOfMethaneInLci(test3) = 2 * 25 = 100.

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

- For the subprocess “test3”:
  \[ \text{amountOfCarbonDioxideInLCIPerProcess(Test3)} \times \text{CharacterisationFactorOfCarbonDioxide} + \text{amountOfMethaneInLCIPerProcess(Test3)} \times \text{CharacterisationFactorOfMethane} = 8 \times 1 + 4 \times 25 = 108 \]

- For Process-specific emissions:
  \[ \text{amountOfCarbonDioxideInLCIPerProcess(ProcessSpecific)} \times \text{CharacterisationFactorOfCarbonDioxide} + \text{amountOfMethaneInLCIPerProcess(ProcessSpecific)} \times \text{CharacterisationFactorOfMethane} = 2 \times 1 + 0 \times 25 = 2 \]

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”.
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:
  - Carbon dioxide: amount(test2UsedInTest1) \times \text{amountOfCarbonDioxideInLCI(test2)} = 3 \times 10 = 30
  - Methane: amount(test2UsedInTest1) \times \text{amountOfMethaneInLCI(test2)} = 3 \times 4 = 12

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

- Carbon dioxide: amountOfCarbonDioxideInLci \times \text{CharacterisationFactorOfCarbonDioxide} = 35 \times 1 = 35
- Methane: amountOfMethaneInLci \times \text{CharacterisationFactorOfMethane} = 12 \times 25 = 300
In the characterized impacts per process (Figure S45) the details of each subprocess: “test2” and “process-specific emission” are calculated:

- Test2: \[\text{amountOfCarbonDioxideInLCI}_{\text{PerProcessOfTest2}} \times \text{CharacterisationFactorOfCarbonDioxide} + \text{amountOfMethaneInLCI}_{\text{PerProcessOfTest2}} \times \text{CharacterisationFactorOfMethane} = 30 \times 1 + 12 \times 25 = 330\]

- Process specific emissions:
  \[\text{amountOfCarbonDioxideInLCI}_{\text{PerProcessOfProcessSpecific}} \times \text{CharacterisationFactorOfCarbonDioxide} + \text{amountOfMethaneInLCI}_{\text{PerProcessOfProcessSpecific}} \times \text{CharacterisationFactorOfMethane} = 5 \times 1 + 0 \times 25 = 5\]

![Figure S45: Characterised impacts, per process, of external process test1](image)

### 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](image)

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 6\(^{th}\) column:

  - Carbon dioxide: amount\_of\_Carbon\_Dioxide\_In\_LCI\_of\_test1 \* amount\_of\_test1\_Used\_In\_Basic \* Energy\_of\_input = 35 \* (-3) \* 4209 = -4.419E5
  - Methane: amount\_of\_Methane\_In\_LCI\_of\_test1 \* amount\_of\_test1\_Used\_In\_Basic \* Energy\_of\_input = 12 \* (-3) \* 4209 = -1.515E5

<table>
<thead>
<tr>
<th>Name</th>
<th>Compartiment</th>
<th>Sub compartment</th>
<th>Unit</th>
<th>Total</th>
<th>Input-specific emissions</th>
<th>Process-specific emissions</th>
<th>test1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide, fossil</td>
<td>air</td>
<td>unspecified</td>
<td>kg</td>
<td>-4.319E+05</td>
<td>0</td>
<td>9999</td>
<td>-4.419E+05</td>
</tr>
<tr>
<td>Methane, fossil</td>
<td>air</td>
<td>unspecified</td>
<td>kg</td>
<td>-1.515E+05</td>
<td>0</td>
<td>0</td>
<td>-1.515E+05</td>
</tr>
</tbody>
</table>

**Figure S47: LCI of basic process**

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

- Carbon dioxide: amount\_of\_Carbon\_Dioxide\_In\_LCI \* Characterisation\_Factor\_Of\_Carbon\_Dioxide = -4.319E5\*1 = -4.319E5
- Methane: amount\_of\_Methane\_In\_LCI \* Characterisation\_Factor\_Of\_Methane = -1.515E5 \* 25 = -3.787E6

<table>
<thead>
<tr>
<th>Name</th>
<th>Compartiment</th>
<th>Sub compartment</th>
<th>IPCC 2007, climate change, GWP 100a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sum</td>
<td></td>
<td></td>
<td>-4.22E+06</td>
</tr>
<tr>
<td>Carbon dioxide, fossil</td>
<td>air</td>
<td>unspecified</td>
<td>-4.319E+05</td>
</tr>
<tr>
<td>Methane, fossil</td>
<td>air</td>
<td>unspecified</td>
<td>-3.788E+06</td>
</tr>
</tbody>
</table>

**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:

- Test1: amount\_of\_Carbon\_Dioxide\_In\_LCI\_Per\_Process\_Of\_Test1 \* Characterisation\_Factor\_Of\_Carbon\_Dioxide + amount\_of\_Methane\_In\_LCI\_Per\_Process\_Of\_Test1 \* Characterisation\_Factor\_Of\_Methane = -4.419E5\*1 + (-1.515E5)\*25 = -4.229E6
- Process specific emissions: amount\_of\_Carbon\_Dioxide\_In\_LCI\_Per\_Process\_Of\_Process\_Specific \* Characterisation\_Factor\_Of\_Carbon\_Dioxide
$e + \text{amountOfMethaneInLciPerProcess(ProcessSpecific)} \times \text{CharacterisationFactorOfMethane} = 9999 \times 1 + 0 \times 25 = 1 \times 10^4$

![Figure S49: Characterised impacts, per process, of basic process](image)

### 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](image)

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
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 multiplying each number in the normalised 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: \(-2.16 \times 10^5\) kg so the weighted impact for the category “IPCC 2007, climate change, GWP 100 a” is: \(-2.16 \times 10^5 \times 10 = -2.16 \times 10^6\) PE
- Methane: \(-1.9 \times 10^6\) kg so normalised impact for the category “IPCC 2007, climate change, GWP 100 a” is: \(-1.9 \times 10^6 \times 10 = -1.9 \times 10^7\) PE

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

Figure S53: Weighted impacts, per substance, 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).

The LCI calculation is for each external process:

\[
\text{LCI} = \text{Total}_\text{amount} \times \frac{\% \text{Percentage}_\text{field}}{100} \times \text{Amount}_\text{PerKgFraction} \times \text{LCI(external process)}
\]

In the example, let’s calculate for test3:

- Carbon dioxide: \(30 \times \frac{70}{100} \times 2 \times 4 = 168 \text{ kg}\)
- Methane: \(30 \times \frac{70}{100} \times 2 \times 2 = 84 \text{ kg}\)

And for test1:

- Carbon dioxide: \(30 \times \frac{30}{100} \times 3 \times 35 = 945 \text{ kg}\)
- Methane: \(30 \times \frac{30}{100} \times 3 \times 12 = 324 \text{ kg}\)

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

\[
\text{sum_for_each_ele_exch} [\text{Total_amount} \times \text{Percentage_field/100} \times \text{AmountPerKgFraction} \times \text{LCI(external_process)} \times \text{characterization_factor(elem. exch)}]
\]

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

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

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

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.

The LCI calculation is for each external process:

\[
\text{Total_amount(MJ)} \times \text{Percentage_field(fraction)/100} / \text{energy%(fraction, MJ/kg)} \times 100/\text{TS%(fraction)} \times \text{AmountPerKgFraction} \times \text{LCI(external_process)}
\]

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: \(30 \times \frac{70}{100} / 18.3 \times \frac{100}{23} \times 2 \times [4 \text{ kg CO}_2; 2 \text{ kg CH}_4] = [39.91 \text{ kg CO}_2; 19.95 \text{ kg CH}_4]\)

**Figure S60: LCI of energy generation process**

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

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

**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.

![Material generation diagram](Image)

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

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

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

<table>
<thead>
<tr>
<th>Fraction name</th>
<th>H (kg)</th>
<th>K (kg)</th>
<th>N (kg)</th>
<th>Na (kg)</th>
<th>O (kg)</th>
<th>P (kg)</th>
<th>S (kg)</th>
<th>Ag (kg)</th>
<th>Al (kg)</th>
<th>As (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vegetable food waste</td>
<td>0.3188</td>
<td>0.06134</td>
<td>0.09177</td>
<td>0.01507</td>
<td>1.908</td>
<td>0.01116</td>
<td>0.000887</td>
<td>0</td>
<td>0.004975</td>
<td>1.265E-06</td>
</tr>
<tr>
<td>Office paper</td>
<td>0.4109</td>
<td>0.0009696</td>
<td>0.008217</td>
<td>0.00636</td>
<td>3.016</td>
<td>0.0003139</td>
<td>0.005284</td>
<td>0</td>
<td>0.01076</td>
<td>1.75E-06</td>
</tr>
</tbody>
</table>

**3.1 Substance transfer per fraction**

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

- For C_fossil, 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.
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).
So the LCI of these Material transfer emissions is calculated for each material property in the dropdown list as: \[ \text{SumForAllFractionsOf} \left[ \text{TransferCoefficientToCompartment}(\text{fraction}) \times \text{AmountProperty}(\text{fraction}) \right] \times \text{ConversionFactorInInterface} \]

So in our example:

- Carbon dioxide, air, unspecified: \(0.15 \times \text{input.cfossil(vegetablefoodwaste)} + 0.02 \times \text{input.cfossil(officepaper)}\) \times \frac{44}{12} = (0.15 \times 0.01154 + 0.02 \times 0.01545) \times \frac{44}{12} = 0.00748 \text{ kg}

- Aluminium, air, unspecified: \(0.4 \times \text{input.al(vegetablefoodwaste)} + 0.4 \times \text{input.al(officepaper)}\) \times 1 = (0.4 \times 0.004975 + 0.4 \times 0.01076) \times 1 = 0.006294 \text{ kg}

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

- Process-specific:
  - Aluminium, air, unspecified: 0.002 \times \text{30} = 0.06
  - Methane fossil, air, unspecified: 0.05 \times \text{30} = 1.5

- Test3: 0.003 \times \text{30} \times \{2 \text{ kg CH}_4; 4 \text{ kg CO}_2\} = \{0.18 \text{ kg CH}_4; 0.36 \text{ kg CO}_2\}.

![Figure S67: LCI of the “substance transfer per fraction” process](image)

![Figure S68: Characterised impacts (subs) of the “substance transfer per fraction” process](image)
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.

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: $\text{TransferCoefficientToCompartment} \times \sum\text{AmountProperty} \times \text{ConversionFactorInInterface}$

So in our example:

- Carbon dioxide, air, unspecified: $0.02 \times (\text{input.cfossil(vegetablefoodwaste)} + \text{input.cfossil(officepaper)}) \times \frac{44}{12} = 0.02 \times (0.01154 + 0.01545) \times 44/12 = 0.001979$ 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:
  - 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}.

Figure S72: LCI of the “substance transfer default” process

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

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.

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
- "Nitrate, water, ground-": (0.09177+0.008217) * 4/100 *(3*15.999+14.007)/14.007 = 0.0177 kg
- "Nitrate, 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 CO2; 2kg CH4} = {240 kg CO2; 120 kg CH4}.

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.

---

**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 kg

Methane, fossil:
amountOfMethaneFossilInLCI*CharacterisationFactorOfMethane = 120*25 = 3000 kg

Methane, non-fossil:
amountOfMethaneNonFossilInLCI*CharacterisationFactorOfMethane = 0.859*25 = 21.47 kg

Dinitrogen monoxide:
amountOfDinitrogenMonoxideInLCI*CharacterisationFactorOfDinitrogenMonoxide = 0.003142*298 = 0.9363 kg

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
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.

The LCI of the emissions happening in the material transfer is calculated for each line as 
\[
\text{amountOfPropertyInInput} \times \text{TransformedAtPercent/100} \times \text{ConversionFactor}
\]
So for our two emissions, it gives:
- Carbon dioxide, fossil, air, unspecified: \(\text{input.Cbio} \times 80/100 \times (-44/12) = -15.72 \text{ kg}\)
- Aluminium, soil, agricultural: \(\text{input.Al} \times 25/100 \times 1 = 0.003935 \text{ kg}\)
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}.

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.

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)*CharacterisationFactorOfCar 
  bonDioxide = -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, their value is given in the Section 3 of this Part III.

1.1 Incineration scenario

Material generation, based on “Material generation” template:

![Material generation diagram]

Collection, based on the “Basic process” template:

![Collection diagram]

Transport, based on the “Basic process” template:

![Transport diagram]
Decrease of energy content due to water evaporation, based on the “Change of energy content” template:

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):

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

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

Transport – 50 km, based on the “Basic process” template:
Landfill leachate generation, based on the “Leachate generation” template:

<table>
<thead>
<tr>
<th>Name</th>
<th>Amount</th>
<th>Unit</th>
<th>Per</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marginal Electricity Consumption incl. Fuel Production, Coal, Energy Quality, DL, kWh, 2006</td>
<td>0.0057</td>
<td>gry, elec</td>
<td>0.001</td>
<td>kWh kg Total Wet Weight</td>
</tr>
</tbody>
</table>

Elementary exchanges: [Add external exchange]

Material transfer

<table>
<thead>
<tr>
<th>Landfill leachate generation</th>
<th>Time period duration (years)</th>
<th>Time horizon of the inventory (in years)</th>
<th>Height of layer (m)</th>
<th>Bulk density (t/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>5</td>
<td>100</td>
<td>20</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Define leachate concentrate (in mg/L)

<table>
<thead>
<tr>
<th>Name</th>
<th>Time period 1</th>
<th>Time period 2</th>
<th>Time period 3</th>
<th>Time period 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>400</td>
<td>150</td>
<td>80</td>
<td>70</td>
</tr>
<tr>
<td>S</td>
<td>0.80</td>
<td>0.015</td>
<td>0.007</td>
<td>0.007</td>
</tr>
<tr>
<td>Si</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>Mg</td>
<td>0.6</td>
<td>0.2</td>
<td>0.1</td>
<td>0.05</td>
</tr>
<tr>
<td>Fe</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Mn</td>
<td>0.007</td>
<td>0.001</td>
<td>0.0001</td>
<td>0.00009</td>
</tr>
<tr>
<td>Zn</td>
<td>0.02</td>
<td>0.015</td>
<td>0.01</td>
<td>0.003</td>
</tr>
<tr>
<td>Na</td>
<td>0.1</td>
<td>0.2</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>K</td>
<td>0.0013</td>
<td>0.0008</td>
<td>0.0003</td>
<td>0.0002</td>
</tr>
<tr>
<td>Ca</td>
<td>500</td>
<td>200</td>
<td>80</td>
<td>35</td>
</tr>
<tr>
<td>Cr</td>
<td>0.0023</td>
<td>0.0004</td>
<td>0.0004</td>
<td>0.0003</td>
</tr>
<tr>
<td>Cu</td>
<td>1.5</td>
<td>0.5</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>Hg</td>
<td>0.0005</td>
<td>0.0002</td>
<td>0.06-05</td>
<td>25-45</td>
</tr>
<tr>
<td>Cd</td>
<td>0.0002</td>
<td>0.06-05</td>
<td>25-45</td>
<td>25-45</td>
</tr>
<tr>
<td>P</td>
<td>0.25</td>
<td>0.13</td>
<td>0.06</td>
<td>0.04</td>
</tr>
<tr>
<td>Na</td>
<td>0.002</td>
<td>0.002</td>
<td>0.002</td>
<td>0.002</td>
</tr>
</tbody>
</table>

Stored ecotoxicity, based on the “Substance transfer – default” template:
Leachate collection, based on the “Mass transfer over years” template:

Waste water treatment plant, based on the “substance transfer – default” template:
Emissions to groundwater, based on the “substance transfer – default” template:
1.2 Anaerobic digestion (AD) scenario

Material generation, based on “Material generation” template:

Collection, based on the “basic process” template:

Transport, based on the “basic process” template:

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

<table>
<thead>
<tr>
<th>Impact category</th>
<th>Method</th>
<th>Unit</th>
<th>Normalisation factor</th>
<th>Year and space of normalisation, reference, remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Climate change</td>
<td>IPCC (Forster et al., 2007)</td>
<td>kg CO2-Eq</td>
<td>7730</td>
<td>Laurent et al., 2011a</td>
</tr>
<tr>
<td>Ozone depletion</td>
<td>EDIP97 (WMO) (Wenzel et al., 1997)</td>
<td>kg CFC-11-Eq</td>
<td>2.05E-2</td>
<td>Laurent et al., 2011a</td>
</tr>
<tr>
<td>Human toxicity, cancer effects</td>
<td>USEtox (Rosenbaum et al., 2008)</td>
<td>CTUh</td>
<td>3.25E-5</td>
<td>Laurent et al., 2011b</td>
</tr>
<tr>
<td>Human toxicity, non-cancer effects</td>
<td>USEtox (Rosenbaum et al., 2008)</td>
<td>CTUh</td>
<td>8.14E-4</td>
<td>Laurent et al., 2011b</td>
</tr>
<tr>
<td>Particulate matter/ respiratory inorganics</td>
<td>Updated from Humbert (2009), from SI of Laurent et al. (2012)</td>
<td>kg PM2.5-eq</td>
<td>4.71</td>
<td>From SI of Laurent et al. (2012)</td>
</tr>
<tr>
<td>Acidification</td>
<td>ReCiPe (Van Zelm et al., 2008)</td>
<td>kg SO2-Eq</td>
<td>49.9</td>
<td>Sleeswijk et al., 2008</td>
</tr>
<tr>
<td>Eutrophication, terrestrial</td>
<td>CML (Guinée et al. 2002)</td>
<td>kg NOx-Eq</td>
<td>356</td>
<td>Huijbregts et al, 2003 and CML(2012) ^3</td>
</tr>
<tr>
<td>Photochemical ozone formation</td>
<td>ReCiPe (Van Zelm et al., 2008)</td>
<td>kg NMVOC</td>
<td>52.9</td>
<td>Sleeswijk et al., 2008</td>
</tr>
<tr>
<td>Eutrophication, freshwater</td>
<td>ReCiPe (Van Zelm et al., 2008)</td>
<td>kg P-Eq</td>
<td>0.69</td>
<td>Sleeswijk et al., 2008</td>
</tr>
<tr>
<td>Ecotoxicity (freshwater)</td>
<td>USEtox (Rosenbaum et al., 2008)</td>
<td>CTUe</td>
<td>5060</td>
<td>Laurent et al., 2011b</td>
</tr>
<tr>
<td>Resource depletion, mineral and fossil</td>
<td>CML(Guinée et al., 2002)</td>
<td>kg antimony-Eq</td>
<td>0.95</td>
<td>Guinée et al., 2002 ^1</td>
</tr>
</tbody>
</table>

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


