

## IEooc\_Methods4\_Exercise6a: Compilation of process inventories for LCA from literature sources

### Sample solution

**Note:** For this exercise an ecoinvent licence for openLCA is needed. If no license is at hand, the exercise can be modified, using the freely available life cycle databases on the openLCA Nexus.

**Task:** Conduct a simple cradle-to-gate analysis of hydrogen production, focussing on climate pressure and primary energy demand. Use foreground data supplied by a literature source (Bareiß et al., 2019). Goal and scope: Here, functional unit and reference flow shall be identical: 1 kg of H<sub>2</sub>, dried, with a standard quality of 5.0 and 30 bar pressure at 60 °C operating temperature.

**Hint:** This exercise is partly a tutorial, so it's recommended to check with the sample solution for this exercise regarding what is expected for the different steps.

### Steps to be taken:

- 1) Define the MEFA process diagram and convert to an LCA flow diagram for the reference flow. (No numbers are needed at this stage.)
- 2) Quantify both the MEFA and the LCA process descriptions with the available data from the main source (Bareiß et al., 2019) for its designed capacity and over its actual lifetime. Use the "near future" technology variant in the reference, cover both the electrolyser (Tables 1 and 2) and the ancillary materials (balance of plant, Table 3) and document your calculations!
- 3) Convert the LCA process description into a unit process for the reference flow 1 kg of H<sub>2</sub>.
- 4) Define the LCA product system (graphical) by linking the electrolyser process (foreground) to a generic background of material and energy supply as well as recycling and waste treatment.
- 5) Transfer your LCA product system description to openLCA+ecoinvent and document this step.

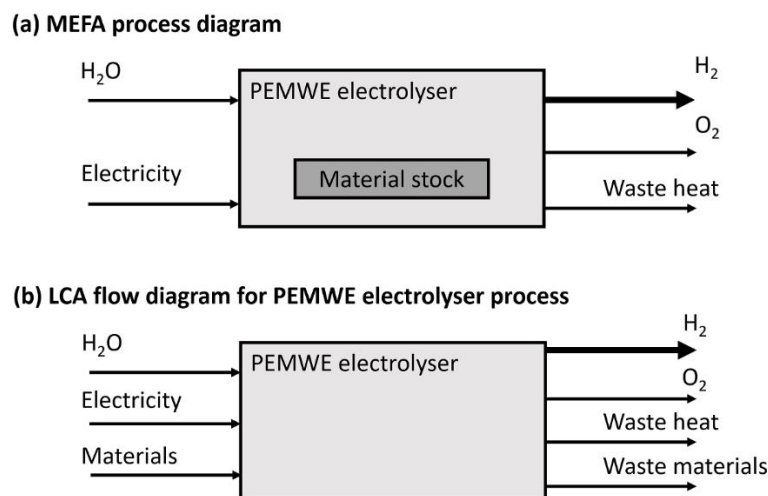
### References

Bareiß, K., de la Rua, C., Möckl, M., & Hamacher, T. (2019). Life cycle assessment of hydrogen from proton exchange membrane water electrolysis in future energy systems. *Applied Energy*, 237, 862–872. <https://doi.org/10.1016/j.apenergy.2019.01.001>

This paper is available open access, the data relevant for this work can be found in Tables 1, 2, and 3.

**Step 1: Define MEFA process diagram and convert to LCA flow diagram**

The reference flow of the LCA product system shall be 1 kg of H<sub>2</sub>, dried, with a standard quality of 5.0 and 30 bar pressure at 60 °C operating temperature. To produce this substance, an electrolyser (here, a PEMWE system (Proton exchange membrane water electrolysis)) is needed, which requires water and electricity as input (Fig. 3 in the main reference Bareiß et al. (2019)). Fig. 3 in Bareiß et al. (2019) can be simplified into the following MEFA process description (Fig. 1a), with two inputs, two outputs plus waste heat to meet the energy balance, and a material stock that represents the actual production asset.



**Figure 1:** MEFA process model and LCA flow diagram of the PEMWE electrolyser process as described in Bareiß (2019). Part (a) is a direct abstraction from the system diagram in Fig. 3 in the paper, where waste heat was added to keep the energy balance and the material stock represents the production assets. Part (b) includes a conversion from the material stocks in the production assets to material flows, understood as average material consumption per amount of hydrogen produced. To keep the mass balance, a corresponding material waste flow must be introduced as well.

In a second step, the MEFA process diagram is converted to an LCA flow diagram (Fig. 1b). This step includes a conversion from the material stocks in the production assets to material flows, understood as average material consumption per amount of hydrogen produced. To keep the mass balance, a corresponding material waste flow must be introduced as well. The background here is that there are no explicit stocks in LCA, but that all stocks are converted into flows whose value corresponds to the amount of main output they generate. For example, if a vehicle (part of the use phase fleet or in-use stock) runs for 200000 km, the provision of 200000 of vehicle transportation will consume exactly one vehicle, modelled as inflow, and produce one end-of-life vehicle, modelled as outflow.

**Step 2: Quantify both the MEFA and the LCA process descriptions with the available data**

For this quantification, the flows and stocks are quantified for the process with its actual capacity and over its actual lifetime: The ‘near future’ option of PEMWE stack described by Bareiß et al. (2019) has a capacity of 1 MW, a lifetime of 90000 h or roughly ten years of continuous service, and a system-wide efficiency of 60% (defined as the lower heating value of the hydrogen produced per electricity consumed). We also know from the text: “From stoichiometry results, we know that 9 kg H<sub>2</sub>O are required for producing 1 kg H<sub>2</sub>. In addition, 55 kWh of electricity are necessary for water splitting at an efficiency of 60% LHV.” The molar mass of H<sub>2</sub>O is roughly 18 g/mol, 2g of which are H<sub>2</sub> and 16 g is oxygen. This information leads to the following values:

**For the MEFA process model:**

**Flows:**

• Water input:	14727 tons	calculated as 9 * mass of H <sub>2</sub>
• Electricity input:	90 GWh	calculated as 1 MW*90000h
• Hydrogen output:	1636.4 tons	calculated as 90 GWh / (55 kWh/kg)
• Oxygen output:	13091 tons	calculated as 8 * mass of H <sub>2</sub>
• Heat loss:	36 GWh	calculated as loss of 100%-60%

**Stocks (not all materials reported are covered)**

• Titanium	37 kg	Table 2
• Stainless steel:	40 kg	Table 2
• Iridium	0.037 kg	Table 2
• Platinum	0.010 kg	Table 2
• Low alloyed steel:	4.8 tons	Table 3
• High alloyed steel:	1.9 tons	Table 3
• Plastics:	0.3 tons	Table 3
• Electronics:	1.1 tons	Table 3
• Concrete:	5.6 tons	Table 3

**For the LCA flow diagram, the stock is converted to an inflow of materials to stock (production phase) and waste flows of the same quantity (end-of-life stage).**

**Inflows:**

• Water input:	14727 tons	calculated as 9 * mass of H <sub>2</sub>
• Electricity input:	90 GWh	calculated as 1 MW*90000h
• Titanium	37 kg	Table 2
• Stainless steel:	40 kg	Table 2
• Iridium	0.037 kg	Table 2
• Platinum	0.010 kg	Table 2

Part II Methods

Methods part 4 (Life cycle assessment)

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- Low alloyed steel: 4.8 tons Table 3
- High alloyed steel: 1.9 tons Table 3
- Plastics: 0.3 tons Table 3
- Electronics: 1.1 tons Table 3
- Concrete: 5.6 tons Table 3

**Outflows:**

- Hydrogen output: 1636.4 tons calculated as 90 GWh / (55 kWh/kg)
- Oxygen output: 13091 tons calculated as 8 \* mass of H<sub>2</sub>
- Heat loss: 36 GWh calculated as loss of 100%-60%
- Waste titanium 37 kg Table 2
- Waste stainless steel: 40 kg Table 2
- Waste iridium 0.037 kg Table 2
- Waste platinum 0.010 kg Table 2
- Waste low alloyed steel: 4.8 tons Table 3
- Waste high alloyed steel: 1.9 tons Table 3
- Waste plastics: 0.3 tons Table 3
- Waste electronics: 1.1 tons Table 3
- Waste concrete: 5.6 tons Table 3

**Step 3: Convert the LCA process description into a unit process for 1 kg H<sub>2</sub>.**

In this step, all flows of the LCA process inventory (step 1) are scaled down to the chosen reference flow of 1 kg H<sub>2</sub> simply by dividing them by the total mass of hydrogen generate over the entire life cycle, which is 1636400 kg:

**Inflows:**

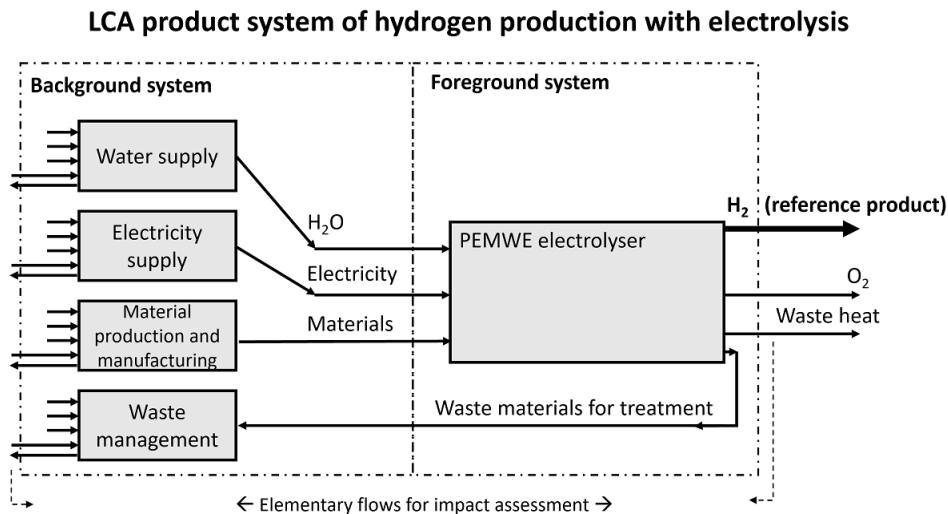
- Water input: 9 kg scaled down from inventory at scale
- Electricity input: 55 kWh scaled down from inventory at scale
- Titanium 0,0226 g scaled down from inventory at scale
- Etc.

**Outflows:**

- **Hydrogen output:** **1 kg** **reference flow by definition**
- Oxygen output: 8 kg scaled down from inventory at scale
- Heat loss: 22 kWh scaled down from inventory at scale
- Waste titanium 0,0226 g scaled down from inventory at scale
- Etc.

#### Step 4: Defining the LCA product system

In the LCA product system (Fig. 2), the electrolyser in the foreground (defined as the part of the product system with custom processes and case study-specific data) is connected to generic process description for supplying the required input flows (water, electricity, materials, ...) and for treating the waste generated. The processes in the background are connected to each other (for a process database) or come as separate life cycle inventories (for an LCI database). Together, foreground and background systems form the product system for the chosen reference flow. In the figure below, all inflows to the foreground system are seen as manufactured goods in a sense that there are connected to industrial activities such as water supply or the electricity grid for their supply. The materials outflow is sent to waste treatment, the hydrogen produced is the reference product, and the by-products waste heat and oxygen are treated as if they left the system for use elsewhere.

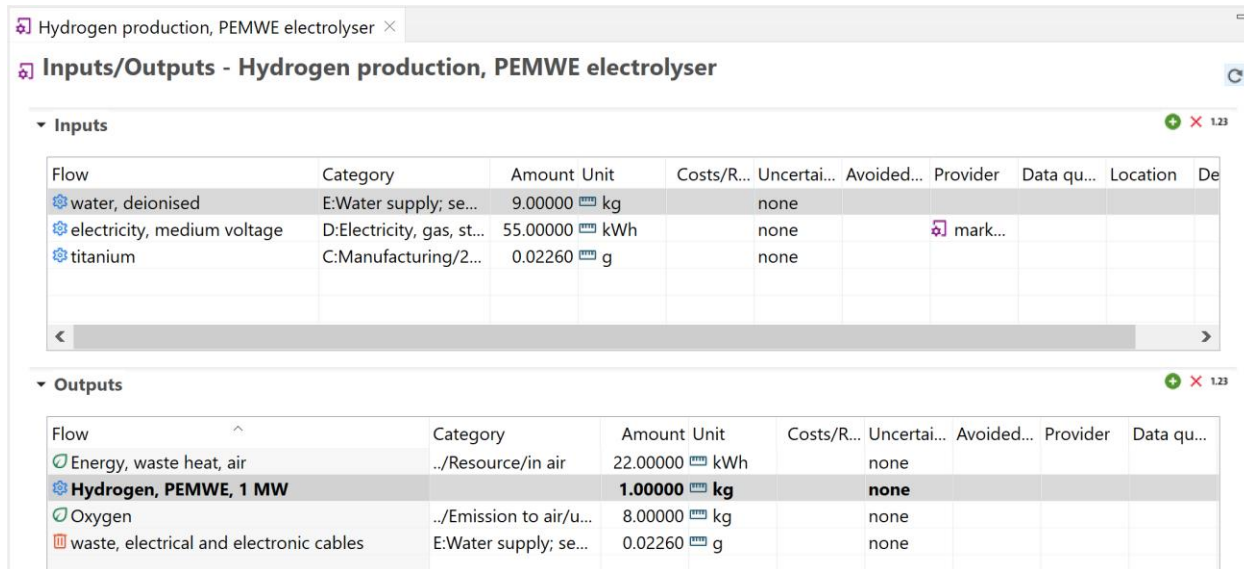


**Figure 2:** LCA product system for hydrogen production with a PEMWE electrolyser.

In this product system version, all impacts will be allocated to the hydrogen and none to the waste heat and oxygen. To achieve a more balanced split of all input requirements across the three outputs, an *allocation* step will be necessary to divide all input requirements to the three products, following a certain breakdown key, based on, e.g., monetary value or exergy content of the three outflows.

**Step 5: Implementation and documentation of the product system in openLCA+ecoinvent.**

In this step, the foreground flows of the product system in Fig. 2 are transferred to openLCA, here with ecoinvent 3.9.1., using the numbers obtained for the unit process inventory in step 3 (Fig. 3, only some flows are shown as example). This step is documented by taking a screenshot of the flow tab of the process, so that the background flows chosen, the values entered, the units of the values, and the type of flows (technosphere, waste, elementary) can be seen.



Flow	Category	Amount	Unit	Costs/R...	Uncertai...	Avoided...	Provider	Data qu...	Location	De
water, deionised	E:Water supply; se...	9.00000	kg		none					
electricity, medium voltage	D:Electricity, gas, st...	55.00000	kWh		none		mark...			
titanium	C:Manufacturing/2...	0.02260	g		none					
<b>▼ Outputs</b>										
Energy, waste heat, air	../Resource/in air	22.00000	kWh		none					
<b>Hydrogen, PEMWE, 1 MW</b>		<b>1.00000</b>	<b>kg</b>		<b>none</b>					
Oxygen	../Emission to air/u...	8.00000	kg		none					
waste, electrical and electronic cables	E:Water supply; se...	0.02260	g		none					

**Figure 3:** Screenshot of a quick openLCA+ecoinvent implementation of the LCA product system for hydrogen production with a PEMWE electrolyser. This implementation shows only some of the flows listed above, as example.

In this unit process description, each input and output flow is linked to an entry in the ecoinvent 3.9.1 background database. The flow types (technosphere, waste, elementary) can clearly be seen, the flow names and providers (where applicable), and the values and units are documented as well. The list of flows in the example is not complete, more of the flows obtained in steps 2 and 3 need to be entered to complete the foreground process description.

Note that during this step, a number of simplifications and assumptions has to be made:

- Choose a specific electricity mix (region!) or a specific provider of a material or product. Possible refinement: Define and model a case study-specific electricity mix, manufacturing process, or material production (e.g., with custom recycled content).
- Co-products are not used but released to the environment without further impact/accounting. Possible refinement: Perform an allocation step (via mass, exergy, or monetary value) to split the different inflows and waste outflows to the different co-products.
- A generic waste treatment process was chosen for a specific material. Possible refinement: Define and describe a case study-specific dismantling and recycling process for certain materials.