**Hydrogen internal combustion engine CHP in decentralized energy systems:   
Towards TEA-LCA in an open-source framework**

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**Life-cycle inventory report**

**For readability and foster transparency, this document regroups and slightly format the notes available in the description cell of the activities created in Activity Browser to create our LCI. They are the same available in the comment cell of the exported Excel files, associated to each of the relevant activities.**

*Content*

[**ICE-CHP flows** 2](#_Toc201162115)

[**PV flows** 6](#_Toc201162116)

[**WT flows** 9](#_Toc201162117)

[**BAT flows** 11](#_Toc201162118)

[**GSHP flows** 12](#_Toc201162119)

[**PEMEL flows** 14](#_Toc201162120)

[**H2C flows** 16](#_Toc201162121)

[**H2S flows** 17](#_Toc201162122)

# **ICE-CHP flows**

**ICE-CHP unit construction, 38kWel+53.7kWth  
common components, electricity components, heat components**

This activity is based on comparison of the ecoinvent 3.10 activities for:

50 kWel, 160 kWel, 200 kWel, 500 kWel, 1 MWel.

* "heat and power co-generation unit construction, X kW electrical, common components for heat+electricity (RER)"

No modification of the lifetime considered.

160kW is the base dataset, and others were extrapolated from it.

We selected the RER equivalent activities instead of the markets.

For all exchanges, we use a power progression following the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098)

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

Based on the 4 previously mentioned extrapolated activities, we can do a fit to determine the extrapolation:

C(X) = a \* Xb

Where:

* C: flow value
* a: regression coefficient across the datasets (not just the ratio of 2 X values)
* X: capacity (here, kW)
* b: scaling factor

All R2 values were above 0.999.

Thus:

* a = 0.0093 & b = 0.9187 for "market for gas motor, 206kW"

So C2 = 0.0093 \* (38)0.9187 = 0.263

* a = 0.0269 & b = 0.6777 for "maintenance, heat and power co-generation unit, 160kW electrical"

So C2 =0.0269 \* (38)0.6777 = 0.316

* a = 0.0381 & b = 0.6126 for the other flows

So C2 = 0.0381 \* (38)0.6126 = 0.354

Based on the operation parameters for our ICE-CHP:

1500 rpm, λ = 2.6 (ultra lean burn), H2 fuel

We can consider to be in the situation where no catalytic converter is needed. Indeed:

* The catalytic converter is present in the 160kWel ecoinvent dataset
* But absent from the extrapolated ones which are based on typical lean operation on natural gas

Ultra lean operation on H2 is comparable to the latter datasets and thus don't require the catalytic converter.

We select the b = 0.6121 case and apply the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098):

C2 = 5 \* (38/160)0.6121 = 2.074

We keep the original ecoinvent uncertainties.

**Electricity/Heat, from 38kWel+53.7kWth ICE-CHP**

Based on the ecoinvent 3.10 activities:

* "heat, central or small-scale, natural gas | heat and power co-generation, natural gas, X kW electrical, lean burn (CH)"
* "electricity, low voltage | heat and power co-generation, natural gas, X kW electrical, lean burn (CH)"

The flow repartition in the dedicated ecoinvent report states that system expansion is avoided to allow comparison per output with other activities. Thus, several allocation alternatives are explored. The allocation choice available in the database is based on exergy. Our system is heat led, so allocation by exergy is not appropriate and should be replaced by allocation based on energy.

The ecoinvent computation for unit use:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

With Electricity & Heat annual yields based on the OpenModelica simulation of Beerlage et al., 2024

(https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator)

= y \* kWp/unit \* kWh/(kWp\*1y)   
= 25 \* 38 \* Electricity annual yield   
= 25 \* 38 \* Electricity annual prod / 38   
= 25 \* Electricity annual prod

= Electricity prod during lifetime (kWh/unit)

Then the reciprocal gives:

Unit consumption per produced Electricity (unit/kWh)

= y \* kWp/unit \* kWh/(kWp\*1y)   
= 25 \* 53.7 \* Heat annual yield   
= 25 \* 53.7 \* Heat annual prod / 53.7   
= 25 \* Heat annual prod

= Heat prod during lifetime (kWh/unit or MJ/unit)

Then the reciprocal gives:

Unit consumption per produced Heat (unit/kWh or unit/MJ)

Due to the modulation mode of the CHP in the Beerlage et al. (2024) OpenModelica simulation, this value changes for each scenario:

|  |  |  |
| --- | --- | --- |
| Scenario | Electricity unit consumption / kWh | Heat unit consumption / MJ |
| 1 | 2.86e-07 | 1.97e-07 |
| 2 | 2.77e-07 | 1.92e-07 |
| 3 | 2.74e-07 | 1.90e-07 |
| 4 | 2.80e-07 | 1.93e-07 |
| 5 | 2.83e-07 | 1.96e-07 |
| 6 | 2.87e-07 | 1.98e-07 |
| 7 | 4.55e-07 | 3.14e-07 |
| 8 | 1.15e-06 | 7.87e-07 |
| 9 | 1.02e-06 | 6.99e-07 |
| 10 | 9.83e-07 | 6.72e-07 |
| 11 | 1.02e-06 | 6.97e-07 |
| 12 | 1.09e-06 | 7.46e-07 |
| 13 | 1.21e-06 | 8.25e-07 |
| 14 | 1.67e-06 | 1.15e-06 |
| 15 | 2.87e-07 | 1.98e-07 |
| 16 | 2.85e-07 | 1.97e-07 |
| 17 | 2.88e-07 | 1.99e-07 |
| 18 | 2.94e-07 | 2.03e-07 |
| 19 | 3.00e-07 | 2.07e-07 |
| 20 | 2.99e-07 | 2.06e-07 |
| 21 | 5.25e-07 | 3.61e-07 |
| 22 | 2.87e-07 | 1.98e-07 |
| 23 | 2.86e-07 | 1.97e-07 |
| 24 | 2.88e-07 | 1.99e-07 |
| 25 | 2.94e-07 | 2.03e-07 |
| 26 | 3.00e-07 | 2.07e-07 |
| 27 | 2.99e-07 | 2.06e-07 |
| 28 | 5.37e-07 | 3.70e-07 |

Natural gas consumption is suppressed as our ICE-CHP is fueled by H2. Values for H2 consumption and Electricity/Heat outputs are taken from the OpenModelica simulation of Beerlage et al. (2024). They do not change that much from scenario to scenario, allowing to go with an average value and triangular uncertainty based on min and max value:

* Electricity H2 use (kg/kWh) = 0.08605 [0.08583–0.08655]
* Heat H2 use (kg/MJ) = 0.01648 [0.01643–0.01650]

**This implies a flow repartition of 83.93 % to Electricity and 16.07 % to Heat, which is used to allocate the rest of the flows.**

Typical lubricating oil use for gas engine is 0.025 [0.01 - 0.05] e-03 kg/ MJ input

LHV of H2 considered in the OpenModelica simulations is 119.88 MJ/kg

Thus oil consumption is 2.997 [1.1988–5.994] e-03 kg / kg H2

*Oil consumption Electricity (kg/kWh)*  
= 2.997 [1.1988–5.994] e-03 \* 0.08605 [0.08583–0.08655]   
= 2.579 [1.029–5.188] e-04

*Oil consumption Heat (kg/MJ)*  
= 2.997 [1.1988–5.994] e-03 \* 0.01648 [0.01643–0.01650]   
= 4.939 [1.969–9.890] e-05

Several biosphere flows are set to 0 to take into account the replacement of natural gas by H2:

*Carbon based fuel related flows:*

* Carbon dioxide, fossil
* Carbon monoxide, fossil
* Methane, fossil
* Sulfur dioxide

*Nitrogen based fuel related flow:*

* Dinitrogen monoxide

Other biosphere flows are adapted:

*Nitrogen oxides:*

In theory, using H2 instead of natural gas has the potential to lead to an increase of NOx emissions.

That being said, the operation parameters of the OpenModelica simulation are based on:

* 1500 rpm engine
* λ = 2.6 (ultra lean burn)

→ NOx emissions becomes very low even in the case of pure H2 combustion (see Heffel 2003, Verhelst & Wallner 2009, Sterlepper et al. 2021). An assumption of NOx emission rate 10 to 50 ppm seems reasonable.

This translates into 0.00255 [0.0001–0.005] kg / kg H2

Thus the computations:

NOx (kg / kWh or MJ) = NOx emission rate (kg / kg H2) \* Electricity or Heat H2 use (kg H2 / kWh or MJ)

*NOx emissions Electricity (kg/kWh)*   
= 0.00255 [0.0001–0.005] \* 0.08605 [0.08583–0.08655]   
= 2.1943 [0.0858–4.3275] e-04

*NOx emissions Heat (kg/MJ)*   
= 0.00255 [0.0001–0.005] \* 0.01648 [0.01643–0.01650]   
= 4.2024 [0.1648–8.25] e-05

This is a conservative estimate: in measurements realized by N. Salim et al. on a 4-cylinder engine (1 cylinder with H2 + 3 cylinders with natural gas, λ = 2.6, 1500 rpm):  
→ NOx levels at arround 100 ppm (94 ppm NO + 4 ppm NO2)

*Particulate Matter, < 2.5 µm:*

Emissions comes from carbon based fuel (absent) and lubricating oil (present). Lubricating oil dominates PM emissions in engines (Worton et al. 2014) so we assume all PM emissions results from it for simplicity.

Using:

* "heat, central or small-scale, natural gas | heat and power co-generation, natural gas, 50kW electrical, lean burn (CH)"
* "electricity, low voltage | heat and power co-generation, natural gas, 50kW electrical, lean burn (CH)"

→ The ratio of PM emissions to lubricating oil consumption is 0.005.

So PM emissions are calculated:

*PM emissions Electricity (kg / kWh)*  
= 0.005 \* Oil consumption Electricity

= 0.005 \* 2.579 [1.029–5.188] e-04

= 1.290 [0.515–2.594] e-06

*PM emissions Heat (kg / MJ)*   
= 0.005 \* Oil consumption Heat

= 0.005 \* 4.939 [1.969–9.890] e-05

= 2.4695 [0.985–4.945] e-07

# **PV flows**

**Photovoltaic slanted-roof installation, 0.9MWp, multi-Si, panel, mounted, on roof**

This activity is based on comparison of the ecoinvent 3.10 activities for 3 kWp and 570 kWp installations.

* "photovoltaic slanted-roof installation, 3kWp, multi-Si, panel, mounted, on roof (CH)"
* "photovoltaic plant construction, 570kWp, multi-Si, on open ground (GLO)"

→ Lifetime : 30 years (no modification compared to the slanted roof installation activity)

Normalized flows per kW installed shows a linear progression for:

* market for photovoltaic mounting system (m2)
* market for photovoltaic panel, multi-Si wafer (m2)

→ Indeed, their normalized ratios = 0.987, equivalent to only 1.3% flow economy with installed capacity

The "electricity, low voltage" flow shows a nonlinear progression:

Indeed, ratio between normalized activities is 0.825, equivalent to 17.5% flow economy with installed capacity.

For this flow, we thus use a power progression following the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098)

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

Based on the 2 previously mentioned activities, we determine a factor b = 0.9632.

So C2 = 0.23 \* (900/3)0.9632 = 55.94

Or C2 = 36.033 \* (900/570)0.9632 = 55.95

We choose:

55.945 kWh and keep the ecoinvent uncertainties

Furthermore, the "market for electricity, low voltage, CH" activity is replaced by the DE version.

Situation is similar (the other way arround) for inverter capacity installed:

* 2.4 \* market for inverter, 2.5 kW => 6 kW
* 3.126 \* market for inverter, 500 kW => 1563 kW

Indeed, ratio between normalized per kWp activities is 1.37, equivalent to 37% flow overuse with installed capacity. The determined factor b=1.0601.

So C2 = 6 \* (900/3)1.0601 = 2536

Or C2 = 1563 \* (900/570)1.0601 = 2536.6

We choose:

2536.3 and keep the ecoinvent uncertainties

This translates into:

5.073 \* market for inverter, 500 kW

Regarding electric installation, where sub-processes are identical:

* Across positive values of sub-process flows:

Log regression gives b = 0.67 with 40.2% deviation

* Removing the polycarbonate extreme outlier:

Log regression gives b = 0.758 with 9.47% deviation

* Further removing the polyvinylchloride of b=0.58:

Log regression gives b= 0.78 with 3.77% deviation

The removed outliers does not seem to have meaningful influence on impacts, as:

Log regression across impact categories gives b = 0.746 with 2.1% deviation.

So C2 = 1 unit \* (900/3)0.746 = 70.46 units of 3 kWp electric installation

Or C2 = 1 unit \* (900/570)0.746 = 1.41 units of 570 kWp electric installation

→ The choice is of no consequence here, so we chose:

70.46 units of 3 kWp electric installation and keep the ecoinvent uncertainties

The "market for diesel, burned in building machine" of the 500 kW plant is not conserved to keep our created activity closer to a slanted roof installation.

**Electricity production, from 0.9MW PV**

The ecoinvent computation:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 30 \* 3 \* annual yield

= 90 \* annual yield

= x kWh/unit

Then the reciprocal should give 1.4447e-05 unit/kWh

So ecoinvent 3.10 annual yield = (1/1.4447e-05)/90 = 771.605 kWh for a 3 kWp unit (reference value).

With Electricity annual yields based on the OpenModelica simulation of Beerlage et al., 2024

(https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator)

* lifetime : 30 years (same as original ecoinvent 3.10 activity)
* annual yield : kWh/(900 kWp \* 1) = 188 294 927.2 / 900 = 209 216.6 kWh for a 0.9MWp unit

So:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 30 \* 900 \* annual yield

= 27000 \* annual yield

= 27000 \* 209 216.6

= 5 648 848 200 kWh/unit

→ Then the reciprocal gives: 1.77e-10 unit/kWh

The "market for tap water" activity is scaled linearly as it should be proportional to the surface of panels, which scales linearly with installed power.

**Photovoltaic slanted-roof installation, 1.8MWp, multi-Si, panel, mounted, on roof**

This activity is based on comparison of the ecoinvent 3.10 activities for 3kWp and 570kWp installations.

* "photovoltaic slanted-roof installation, 3kWp, multi-Si, panel, mounted, on roof (CH)"
* "photovoltaic plant construction, 570kWp, multi-Si, on open ground (GLO)"

→ Lifetime : 30 years (no modification compared to the slanted roof installation activity)

Normalized flows per kW installed shows a linear progression for:

* market for photovoltaic mounting system (m2)
* market for photovoltaic panel, multi-Si wafer (m2)

→ Indeed, their normalized ratios = 0.987, equivalent to only 1.3% flow economy with installed capacity

The "electricity, low voltage" flow shows a non linear progression:

Indeed, ratio between normalized activities is 0.825, equivalent to 17.5% flow economy with installed capacity.

For this flow, we thus use a power progression following the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098)

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

Based on the 2 previously mentioned activities, we determine a factor b = 0.9632.

So C2 = 0.23 \* (1800/3)0.9632 = 109.05

Or C2 = 36.033 \* (1800/570)0.9632 = 109.07

We choose:

109.06 kWh and keep the ecoinvent uncertainties

Furthermore, the "market for electricity, low voltage, CH" activity is replaced by the DE version.

Situation is similar (the other way arround) for inverter capacity installed:

* 2.4 \* market for inverter, 2.5 kW => 6 kW
* 3.126 \* market for inverter, 500 kW => 1563 kW

Indeed, ratio between normalized per kWp activities is 1.37, equivalent to 37% flow overuse with installed capacity. The determined factor b = 1.0601.

So C2 = 6 \* (1800/3)1.0601 = 5287.73

Or C2 = 1563 \* (1800/570)1.0601 = 5288.96

We choose:

5288.35 and keep the ecoinvent uncertainties

This translates into:

10.577 \* market for inverter, 500kW

Regarding electric installation, where sub-processes are identical:

* Across positive values of sub-process flows:

Log regression gives b = 0.67 with 40.2% deviation

* Removing the polycarbonate extreme outlier:

Log regression gives b = 0.758 with 9.47% deviation

* Further removing the polyvinylchloride of b=0.58:

Log regression gives b = 0.78 with 3.77% deviation

The removed outliers does not seem to have meaningful influence on impacts, as:

Log regression across impact categories gives b = 0.746 with 2.1% deviation

So C2 = 1 unit \* (1800/3)0.746 = 118.17 units of 3 kWp electric installation

Or C2 = 1 unit \* (1800/570)0.746 = 2.36 units of 570 kWp electric installation

→ The choice is of no consequence here, so we chose:

118.17 units of 3kWp electric installation and keep the ecoinvent uncertainties

The "market for diesel, burned in building machine" of the 500 kW plant is not conserved to keep our created activity closer to a slanted roof installation.

**Electricity production, from 1.8MW PV**

The ecoinvent computation:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 30 \* 3 \* annual yield

= 90 \* annual yield

= x kWh/unit

Then the reciprocal should give 1.4447e-05 unit/kWh

So ecoinvent 3.10 annual yield = (1/1.4447e-05)/90 = 771.605 kWh for a 3 kWp unit (reference value).

With Electricity annual yields based on the OpenModelica simulation of Beerlage et al., 2024

(https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator)

* lifetime : 30 years (same as original ecoinvent 3.10 activity)
* annual yield : kWh/(1800 kWp \* 1) = 376 589 854.5 / 1800 = 209 216.4 kWh for a 1.8MWp unit

So:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 30 \* 1800 \* annual yield

= 54000 \* annual yield

= 57000 \* 209 216.4

= 11 925 334 800 kWh/unit

→ Then the reciprocal gives: 8.386e-11 unit/kWh

The "market for tap water" activity is scaled linearly as it should be proportional to the surface of panels, which scales linearly with installed power.

# **WT flows**

**Wind power plant construction, 0.5MW**

Scaling from original ecoinvent 3.10 activities:

* "wind power plant construction, 800kW, fixed parts"
* "wind power plant construction, 800kW, moving parts"

We use the approach of Zhang et al. 2017 (DOI: 10.1016/j.apenergy.2016.12.098):

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

We determined a factor b = 0.83 through a phenomenological approach:

We performed a comparative analysis of the evolution of impacts (for every EF impact category, IW footprint category, and Crustal Scarcity indicator) and LCIs.

For these ecoinvent activities:

* wind power plant construction, 800kW (sum of fixed and moving parts), GLO
* wind turbine construction, 750kW, GLO
* wind turbine construction, small-scale, 6kW, DE

Least-square regression on log transformed data was used to determine the best b factor.

* Analysis from the LCIs was usually missing datapoints because they were few exact matching entries across datasets. Fit was rather acceptable (R² between 0.7 and 0.9), with RMSE in log-space being 0.9753.

In this case, b = 0.7387

* When implementing of a fuzzy matching of activities, we obtained a rather poor fit (R² <0.7).  
  RMSE in log-space was 3.1169.

In this case, b = 0.8652

* Analysis from the impacts had sufficient datapoints, with an excellent fit (R² ≥ 0.9).  
  RMSE in log-space was 0.4305.

In this last case, b = 0.8288

→ By selecting b = 0.83, we ensure the 500 kW dataset we create will yield impact results that will be consistent with the 800 kW ecoinvent dataset.

So:

C2/C1 = (X2/X1)b

1 unit (500 kW) = (500/800)0.83 \* 1 unit (800 kW)

Hence:

1 unit (500 kW) = 0.677 unit (800 kW)

Triangular uncertainty was set using:

* b = 1 (linear scaling)

→ 0.625 min

* b = 0.74 (estimation from technosphere comparison for 6, 750, 800 kW datasets, in exact matching case)

→ 0.71 max

**Electricity production, from 0.5MW WT (high voltage)**

This activity was created by adaptation of the "electricity production, wind, <1MW turbine, onshore (DE)" in ecoinvent 3.10.

The ecoinvent computation:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 20 \* 800 \* annual yield

= 16000 \* annual yield

= x kWh/unit

Then the reciprocal should give 3.9007e-08 unit/kWh

So ecoinvent 3.10 annual yield = (1/3.9007e-08)/16000 = 1602.3 kWh for a 0.8 MWp unit (reference value).

One should note there is a discrepancy between this ecoinvent activity (20 years lifetime for both fixed and moving parts) and the presented lifetime of fixed parts in the dedicated dataset, which is supposed to be 40 years according to the ecoinvent documentation at time of work (beginning of 2025).

With Electricity annual yields based on the OpenModelica simulation of Beerlage et al., 2024

(https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator):

* lifetime : 20 years (same as original ecoinvent 3.10 activity for moving parts)
* annual yield : kWh/(500 kWp \* 1) = 413 605.0 / 500 = 827.21 kWh for a 0.5MWp unit

So:

lifetime \* capacity \* annual yield = y \* kWp/unit \* kWh/(kWp\*1y)

= 20 \* 500 \* annual yield

= 10000 \* annual yield

= 10000 \* 827.21

= 8 272 100 kWh/unit

→ Then the reciprocal gives: 1.2089e-7 unit/kWh

The activities associated to lubricating oil were left unchanged as they do not vary between the following ecoinvent datasets:

* electricity production, wind, <1MW turbine, onshore
* electricity production, wind, >3MW turbine, onshore

→ This suggest the value does not vary much for installations between 800 kW and 4.5 MW, thus for a 500 kW installation.

Transportation activity was therefore also left unchanged

**Electricity production, from 0.5MW WT (low voltage)**

Using the ecoinvent 3.10 database for electricity production coming from wind turbine onshore.

Conversion factor accounting for the transformation from high to low voltage:

1.03786932562588 (high) to 1 (low)

This corresponds to the product of the losses from high to medium then medium to low transformation, based on the ecoinvent activities:

* electricity voltage transformation, residual mix, from high to medium voltage
* electricity voltage transformation, residual mix, from medium to low voltage

No uncertainty defined.

# **BAT flows**

**Market for battery, Li-ion, NMC811, rechargeable, prismatic**

This activity is based on the "market for battery, Li-ion, NMC811, rechargeable, prismatic" ecoinvent activity.

As mentioned in the ecoinvent documentation:

Specific energy density is 0.149 kWh/kg of battery at the pack level, based on Dai et al. (2017, 2018, 2019) for battery electric vehicle.

With Storage capacity required based on the OpenModelica simulation of Beerlage et al., 2024

(https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator):

Coefficient applied is then:

500/0.149 = 3355.7

**Market for used Li-ion battery**

This activity is based on the "market for used Li-ion battery" ecoinvent activity

The rest of description is identical to the previous section.

**Electricity, from 500kWh BAT**

Based on OpenModelica simulation of Beerlage et al., 2024

https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator):

* Lifetime : 2600 +- 1000 full cycles / unit
* SOC variation across scenarios : 49.7 ± 0.3 % of installed capacity
* C-rate variation across scenarios : < 0.4

→ medium to low stress on the NMC811 battery

The number of full cycles is usually defined based on a relative capacity degradation (RCD) of 20% compared to beginning of life (BoL) capacity value. Capacity of installed battery: 500 kWh.

A full cycle is when:

* SOC varies from 0.10 to 0.90, then goes back to 0.10
* DoD varies between 0.90 and 0.10, then goes back to 0.90

→ So 80% of the installed capacity in kWh is used to compute the actual throughput.

Over the lifetime, that corresponds to:

* 2500 \* 0.8 \* 500 = 1 000 000 kWh/unit
* 2600 \* 0.8 \* 500 = 1 040 000 kWh/unit
* 2700 \* 0.8 \* 500 = 1 080 000 kWh/unit

Then the reciprocal gives:

* 1.0e-06 unit/kWh
* 9.615e-07 unit/kWh
* 9.259e-07 unit/kWh

The min and max values are used to set triangular uncertainty.

# **GSHP flows**

**Heatpump production, 197kW GSHP**

Values based on the "heat pump production, brine-water, 10kW (CH)" ecoinvent activity.

Original flows correspond to a 10kW GSHP. Flows are linearly scaled to correspond 197 kW GSPH.

Scaling coefficient used:

197/10 = 19.7

Electricity, gas consumption, and plastic waste were set to the DE ecoinvent activity to tailor the model to a German production.

**Borehole heat exchangers production, 150m, for 197kW GSHP**

Values based on the "borehole heat exchanger production, 150m (CH)" ecoinvent activity. The rest of the description is identical to the previous section.

**Heat production, from 197kW GSHP**

Values based on the "heat production, borehole heat exchanger, brine-water heat pump 10kW (CH)" ecoinvent activity.

Lifetimes of infrastructures was kept identical.

* 50 years for borehole heat exchanger and 20 years for heatpump.
* Typical operation mode is 2000 operating hours.

Thus the corresponding normalized flows for a 197 kW heatpump (electricity excepted), postulating the refrigerant is only dependant on the produced heat:

For 1 MJ (electricity excepted):

|  |  |  |  |
| --- | --- | --- | --- |
| technosphere | 1.48e-08 | unit | borehole heat exchangers production |
| 3.53e-08 | unit | heatpump production |
| 2.5e-06 | kilogram | market for refrigerant R134a |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| biosphere | 2.5e-06 | kilogram | 1,1,1,2-Tetrafluoroethane | air - urban air close to ground |
| 0.744 | megajoule | Energy, geothermal, converted |  |

A treatment of heatpump activity, with the same unit consumption as heatpump production, is added to the original activity to take the end-of-life into account.

Flow values per scenario, with Heat in MJ and other values corresponding to electricity in kWh:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Scenario | Heat | CHP->HP | WT->HP | PV->HP | BAT->HP | GRID->HP |
| 1 | 680646.64 | 13012.7 | 9373.8 | 25374.0 | 5223.4 | 9594.5 |
| 2 | 659738.05 | 13851.4 | 9213.2 | 24668.8 | 5188.5 | 7255.2 |
| 3 | 651720.13 | 14271.6 | 8447.5 | 24860.9 | 5018.4 | 6692.9 |
| 4 | 665639.17 | 13367.7 | 8500.1 | 25326.1 | 5111.5 | 8311.6 |
| 5 | 674320.21 | 12733.5 | 8580.7 | 25311.4 | 5285.9 | 9524.5 |
| 6 | 683229.02 | 11158.6 | 8760.8 | 24033.6 | 5469.6 | 12913.5 |
| 7 | 951394.93 | 2444.4 | 14547.7 | 24023.6 | 7488.3 | 39154.3 |
| 8 | 1227110.11 | 3498.9 | 33513.9 | 0.0 | 5197.4 | 70137.5 |
| 9 | 1203943.32 | 4518.8 | 31725.0 | 0.0 | 4681.9 | 69299.7 |
| 10 | 1195660.22 | 2868.4 | 27735.9 | 0.0 | 4462.7 | 74154.4 |
| 11 | 1203414.55 | 2661.5 | 27433.7 | 0.0 | 4252.6 | 75453.8 |
| 12 | 1216990.37 | 2437.7 | 27325.2 | 0.0 | 4077.3 | 76940.2 |
| 13 | 1235389.75 | 1807.4 | 27240.2 | 0.0 | 4079.7 | 79184.3 |
| 14 | 1284537.13 | 984.7 | 29721.9 | 0.0 | 3856.2 | 81898.3 |
| 15 | 682966.48 | 16926.8 | 0.0 | 25801.1 | 5331.7 | 14731.6 |
| 16 | 679843.33 | 16987.2 | 0.0 | 25617.9 | 5317.6 | 13978.2 |
| 17 | 687036.13 | 17656.5 | 0.0 | 27153.1 | 5252.5 | 12499.3 |
| 18 | 701646.73 | 16589.2 | 0.0 | 27691.5 | 5434.3 | 14383.0 |
| 19 | 714977.53 | 15027.4 | 0.0 | 27179.7 | 5835.6 | 17365.3 |
| 20 | 712220.40 | 13186.9 | 0.0 | 24394.9 | 5865.9 | 21674.7 |
| 21 | 1011633.44 | 2497.2 | 0.0 | 24359.0 | 8757.2 | 57297.2 |
| 22 | 682966.48 | 18634.6 | 0.0 | 25865.5 | 0.0 | 18291.2 |
| 23 | 680423.29 | 18665.8 | 0.0 | 25672.7 | 0.0 | 17603.9 |
| 24 | 685635.01 | 19785.0 | 0.0 | 27472.1 | 0.0 | 15156.2 |
| 25 | 700616.77 | 18241.8 | 0.0 | 27588.9 | 0.0 | 18159.0 |
| 26 | 714834.61 | 16944.7 | 0.0 | 27436.3 | 0.0 | 21023.2 |
| 27 | 712636.81 | 14735.0 | 0.0 | 24438.1 | 0.0 | 25997.1 |
| 28 | 1020745.84 | 2864.9 | 0.0 | 24421.1 | 0.0 | 66443.9 |

The Heat value produced (MJ) is thus used to scale the refrigerant, unit consumption, and biosphere flows.

Associated electricity consumptions are used for electricity flows. It can be noted that the heatpump is sparsly used in some scenarios, compared to the typical 2000 operating hours postulated in ecoinvent dataset.

# **PEMEL flows**

**Electrolyzer production, 0.5MWe, PEM, BoP**

This dataset has been adapted from the work of Gerloff 2021 (DOI: 10.1016/j.est.2021.102759)

The scaling approach in this work follow the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098)

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

For Stack components, b=0.7 was used by Gerloff 2021 to scale their LCI to 1 MW. We use the same b coefficient to scale down the LCI for our 0.5 MW electrolyzer.

So:

C2/C1 = (X2/X1)b

0.5 MW flow = (0.5)0.7 \* 1 MW flow

No specific uncertainty is associated to any flow of this PEMEC LCI.

**Electrolyzer production, 0.5MWe, PEM, Stack**

This dataset has been adapted from the work of Gerloff 2021 (DOI: 10.1016/j.est.2021.102759)

The scaling approach in this work follow the approach of Zhang et al. 2017   
(DOI: 10.1016/j.apenergy.2016.12.098)

C2/C1 = (X2/X1)b

With:

* C1: known flow of component 1
* C2: unknown flow of component 2
* X1: capacity (here, kW) of plant, equipment, or component 1
* X2: capacity (here, kW) of plant, equipment, or component 2
* b: scaling factor

For Stack components, b=0.88 was used by Gerloff 2021 to scale their LCI to 1 MW. We use the same b coefficient to scale down the LCI for our 0.5 MW electrolyzer.

So:

C2/C1 = (X2/X1)b

0.5 MW flow = (0.5)0.88 \* 1 MW flow

There is no dedicated flow for iridium in the ecoinvent 3.10 database. The iridium flow has thus been reproduced from Gerloff 2021. Moreover, no uncertainty is associated to any flow of the PEMEC LCI. However, a 30% triangular uncertainty was added on the platinum flow during the LCI implementation in the premise library for the brightway LCA framework. We thus also implemented this triangular uncertainty.

**H2 production, from PEMEL**

This dataset has been adapted from:

* the work of Gerloff 2021 (DOI: 10.1016/j.est.2021.102759)
* and its reprisal in the premise library by Sacchi et al. 2022 (DOI: 10.1016/j.rser.2022.112311)

Here is the orginal dataset for 1 kg H2 produced (electricity excluded, as we're using the OpenModelica simulation of Beerlage et al. 2024 for the electricity flows):

|  |  |  |  |
| --- | --- | --- | --- |
| technosphere | 1.34989e-06 | unit | electrolyzer, 0.5MWe, PEM, Stack |
| 3.37473e-07 | unit | electrolyzer, 0.5MWe, PEM, Balance of Plant |
| -1.34989e-06 | unit | used fuel cell stack, 0.5MWe, PEM |
| -3.37473e-07 | unit | used fuel cell balance of plant, 0.5MWe, PEM |
| 14.0 | kilogram | water, deionized |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| biosphere | 8.0 | kilogram | Oxygen | air |
| 0.000607 | square meter-year | Occupation, industrial area | natural resource - land |
| 3.04e-05 | square meter | Transformation, from industrial area | natural resource - land |
| 3.04e-05 | square meter | Transformation, to industrial area | natural resource - land |

As it can be seen, the H2O quantity is 14 kg. This is 1.55 times superior to the stoichiometric requirement of 9 kg H2O for 1 kg H2. This quantity is associated to the needed water for cooling.

We scale these flows based on the H2 production per scenario in kg and associated electricity flows in kWh:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Scenario | H2 (kg) | CHP->PEMEL | WT->PEMEL | PV->PEMEL | BAT->PEMEL |
| 1 | 16234.13 | 25828.9 | 108582.3 | 955011.6 | 23580.2 |
| 2 | 13847.65 | 25650.7 | 101748.0 | 800343.7 | 21644.4 |
| 3 | 11799.9 | 24284.7 | 79871.0 | 685943.4 | 18895.2 |
| 4 | 11647.54 | 20643.9 | 63533.9 | 698146.5 | 16224.3 |
| 5 | 11384.48 | 22911.2 | 74984.4 | 664875.8 | 17742.3 |
| 6 | 11056.65 | 25089.5 | 73746.2 | 639704.3 | 19497.9 |
| 7 | 8435.9 | 16145.9 | 66402.3 | 481970.9 | 13841.7 |
| 8 | 3372.68 | 7149.0 | 190182.0 | 0.0 | 33898.2 |
| 9 | 3466.83 | 10550.3 | 193719.1 | 0.0 | 33414.6 |
| 10 | 3628.35 | 15444.9 | 200226.3 | 0.0 | 33086.7 |
| 11 | 3434.07 | 15988.9 | 189210.0 | 0.0 | 30239.1 |
| 12 | 3198.73 | 15862.1 | 176049.3 | 0.0 | 27391.5 |
| 13 | 2883.48 | 16403.2 | 157617.9 | 0.0 | 23669.0 |
| 14 | 2073.5 | 14064.5 | 110898.7 | 0.0 | 17194.9 |
| 15 | 15710.71 | 14936.2 | 0.0 | 1051227.9 | 10953.2 |
| 16 | 13044.35 | 14149.1 | 0.0 | 869640.7 | 10523.2 |
| 17 | 10985.81 | 13633.7 | 0.0 | 729688.6 | 9858.4 |
| 18 | 10873.49 | 11403.0 | 0.0 | 725743.8 | 8333.3 |
| 19 | 10637.4 | 12568.8 | 0.0 | 707948.8 | 8776.6 |
| 20 | 10370.02 | 14729.4 | 0.0 | 686101.5 | 10132.1 |
| 21 | 7834.35 | 7009.5 | 0.0 | 524955.6 | 5153.2 |
| 22 | 15686.12 | 20620.9 | 0.0 | 1054810.5 | 0.0 |
| 23 | 13027.49 | 20481.5 | 0.0 | 872675.8 | 0.0 |
| 24 | 10977.25 | 20712.3 | 0.0 | 731881.3 | 0.0 |
| 25 | 10852.35 | 17625.6 | 0.0 | 726405.3 | 0.0 |
| 26 | 10605.71 | 19099.8 | 0.0 | 708021.6 | 0.0 |
| 27 | 10354.39 | 20860.1 | 0.0 | 689031.1 | 0.0 |
| 28 | 7935.67 | 4860.7 | 0.0 | 539204.5 | 0.0 |

Note: the expected lifetime is 20 years with 8000 annual operating hours.

Due to the control sequence in the OpenModelica simulation, the electrolyzer is sparsely used (200–5000 h).

# **H2C flows**

**Hydrogen, from H2C**

Values based on: Ghandehariun and Kumar, 2016 (DOI 10.1016/j.ijhydene.2016.04.077).

Their original energy consumption is calculated based on the exit pressure of the compressor which is considered to be 60 bar. Their compressor has an efficiency of 70% and lifetime of 22 years.

For 1 kg H2 compressed:

|  |  |  |  |
| --- | --- | --- | --- |
| technosphere | 0.00134 | kilogram | steel, chromium steel 18/8, hot rolled |
| 0.000423 | kilogram | cast iron |
| 4.94e-06 | kilogram | ethylene glycol |
| 1.27e-05 | kilogram | lubricating oil |
| 4.23e-05 | kilogram | aluminium, wrought alloy |
| 1.06e-05 | kilogram | tube insulation, elastomere |
| 3.17e-05 | kilogram | copper, cathode |

These values are scaled by the value of H2 flow in kg compressed per scenario. Electricity requirements were excluded and added separately per scenario (based on OpenModelica simulation of Beerlage et al., 2024, https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator)

Note: the compressor used has a 80% efficiency and compress H2 to 80 bar. These differences with Ghandehariun and Kumar, 2016 are neglected regarding the technosphere flows outlined above.

Thus the H2 flows in kg and associated electricity flows in kWh per scenario:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Scenario | H2 comp. & stored | CHP->H2C | WT->H2C | PV->H2C | BAT->H2C |
| 1 | 10705.2 | 2398.3 | 10082.4 | 88677.4 | 2189.5 |
| 2 | 8388.9 | 2381.8 | 9447.8 | 74315.8 | 2009.8 |
| 3 | 6766.9 | 2254.9 | 7416.4 | 63693.1 | 1754.5 |
| 4 | 6765.9 | 1916.9 | 5899.4 | 64826.3 | 1506.5 |
| 5 | 6374.8 | 2127.4 | 6962.7 | 61736.9 | 1647.5 |
| 6 | 5833.1 | 2329.7 | 6847.7 | 59399.6 | 1810.5 |
| 7 | 4387.7 | 1499.2 | 6165.8 | 44753.3 | 1285.3 |
| 8 | 2873.0 | 663.8 | 17659.3 | 0.0 | 3147.6 |
| 9 | 2613.0 | 979.6 | 17987.8 | 0.0 | 3102.7 |
| 10 | 2317.1 | 1434.1 | 18592.0 | 0.0 | 3072.3 |
| 11 | 2047.8 | 1484.6 | 17569.1 | 0.0 | 2807.8 |
| 12 | 1784.0 | 1472.9 | 16347.0 | 0.0 | 2543.4 |
| 13 | 1364.3 | 1523.1 | 14635.6 | 0.0 | 2197.8 |
| 14 | 714.8 | 1306.0 | 10297.5 | 0.0 | 1596.6 |
| 15 | 11293.5 | 1386.9 | 0.0 | 97611.6 | 1017.1 |
| 16 | 8813.7 | 1313.8 | 0.0 | 80750.3 | 977.1 |
| 17 | 7146.4 | 1266.0 | 0.0 | 67755.1 | 915.4 |
| 18 | 7117.5 | 1058.8 | 0.0 | 67388.8 | 773.8 |
| 19 | 6677.4 | 1167.1 | 0.0 | 65736.4 | 814.9 |
| 20 | 5906.8 | 1367.7 | 0.0 | 63707.8 | 940.8 |
| 21 | 4401.1 | 650.9 | 0.0 | 48744.6 | 478.5 |
| 22 | 11315.3 | 1914.8 | 0.0 | 97944.2 | 0.0 |
| 23 | 8829.2 | 1901.8 | 0.0 | 81032.1 | 0.0 |
| 24 | 7205.7 | 1923.2 | 0.0 | 67958.7 | 0.0 |
| 25 | 7081.7 | 1636.6 | 0.0 | 67450.2 | 0.0 |
| 26 | 6698.8 | 1773.5 | 0.0 | 65743.2 | 0.0 |
| 27 | 5914.8 | 1937.0 | 0.0 | 63979.8 | 0.0 |
| 28 | 4518.0 | 451.3 | 0.0 | 50067.7 | 0.0 |

# **H2S flows**

**Hydrogen storage use**

This activity is based on the "storage production, 10'000 l" ecoinvent activity. The original product in ecoinvent is assumed to undergo 100 000 h of operation, which translates in 11-12 years. As the data is quite old, we change the assumption to 20 years, following the value considered in the OpenModelica simulation.  
(Beerlage et al., 2024. https://github.com/IKKUengine/CO2InnO-H2-CHP-Demonstrator)

For 10 m3 volume storage:

0.1 "storage production, 10'000 l" used

1/20 = 0.05 unit use per year

So unit comsumption of storage for a year of the energy system is:

0.1 \* 0.05 = 0.005

For 1000 m3 volume storage:

100 "storage production, 10'000 l" used

1/20 = 0.05 unit use per year

So unit comsumption of storage for a year of the energy system is:

100 \* 0.05 = 5

The same logic is applied for every H2S storage capacity.