Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Electronic Supplementary Information (ESI)

Life cycle assessment of PEM FC applications: electric mobility and µ-CHP.

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MWCNT - Product specification

The multiwalled carbon nanotubes (MWCNT) used for in this case study appears as a black powder. It is a bulk material that forms agglomerates from 1mm to 1 cm on average. The MWCNT form 10 to 20 tubes have a diameter of 15-35 nm and a length bigger than 10 µm. The MWCNT are highly pure (97% MWCNT). The residual 3% of the product represent the catalyst. The MWCNT have a density of 1.4 g/cm^3. There is almost no amorphous carbon present in the product [1, 2]. In order to get MWCNT suitable for electrocatalyst applications, the raw material have to be treated with an acid in order to remove the catalyst and add carboxyl groups on the outer surface of the tube, as first step of further functionalization (acid treatment), and then they have to be functionalised so that the MWCNT achieve the desired surface properties (Figure S1).

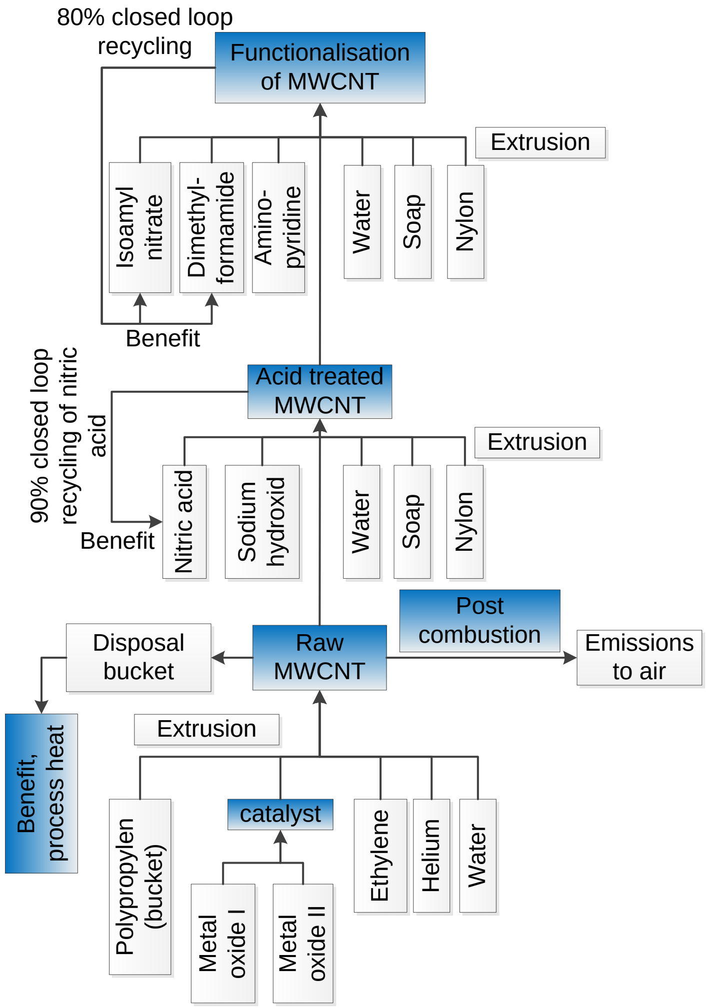


Figure S1. Product system overview for the production of multiwalled carbon nanotubes (MWCNT) including acid treatment and functionalisation. Blue boxes refer to unit processes developed for this case study, white boxes are taken unaltered from ecoinvent.

Most of the data gathered for the life cycle inventory (LCI) of MWCNT production stem from Nanothinx S.A. Although the production process is still on lab scale the data represents industrial technology. To assure that the LCI represents technology on industrial scale some assumptions for up scaling have been taken. This allows a fair comparison with the reference product carbon black (CB).

Unit process: Raw MWCNT

The MWCNTs production reaction takes place in a pilot plant. The production process is a batch process using chemical vapour deposition (CVD) to convert ethylene as a hydrocarbon feedstock into MWCNT. The production of MWCNT is characterised by heating up pure ethylene in quartz tube to about 700°C in an inert helium atmosphere. The ethylene converts into MWCNT when two metal oxides are added as catalyst. The two metal oxides and the amount of each is the secret of the company and therefore the data remain unpublished. Anyway, the environmental impact measured in ReCiPe points of the two metals is below 0.2% compared to the overall impacts of the MWCNT.

The CNT grow only on the catalyst. The conversion factor of ethylene into MWCNT is 70%. The most sensitive part of the technology refers to the catalyst that is used for the MWCNT production. This information is kept secret by the manufacturer. Hence, instead of the exact catalyst which bases on aluminium oxide and iron oxide, a mixture of 50% aluminium oxide and 50% magnetite is used. Polypropylene is used to produce the bucket for shipping the raw MWCNT. The heat production from the disposal of the bucket in a MSWI plant is directly deducted from the process heat required for the MWCNT production process.

The ethylene conversion is about 70%. The rest of the fuel is assumed to be sent to a post combustion process. This process is represented with the emissions profile based on a combined heat and power plant (small scale)[3]. The emission of sulphur dioxide was neglected since there is no possibility that a sulphur containing compound gets into the system. All other emissions (NO_x, CO, CO_2, methane, non-methane volatile organic compounds, N_2O, Particulates) are adjusted reflecting the amount of ethylene into the process. The complete LCI is presented in Table S1.

Table S1. LCI for the production process of raw multiwalled carbon nanotubes (MWCNT).

Production of raw MWCNT			
Imputs	**Amount**	**unit**	**Remark**
Ethylene, average, at plant/RER U	1.4E+00	kg	Carbon feedstock, 70 % conversion
Metal oxide I	unpublished		Representing the catalyst
Metal oxide II	unpublished		
Helium, at plant/GLO U	2.3E-02	kg	For inert atmosphere, amount reflects 2 times the volume of the quartz tube
Polypropylene, granulate, at plant/RER U	5.6E-01	kg	For the bucket
Extrusion, plastic film/RER U	5.4E-01	kg	For the bucket
Water, ultrapure, at plant/GLO U	5.0E+00	kg	Cleaning of the devices, estimate Nanothinx
Electricity, low voltage, production RER, at grid/RER U	2.4E+01	kWh	Measure Nanothinx
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	1.1E+00	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	2.6E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
MWCNT, raw, at plant	1.0E+00	kg	Final product
Nitrogen oxides to air	4.2E-04	kg	Emissions profile based on a small scale combined heat and power plant
Carbon monoxide to air	2.4E-03	kg	Emissions profile based on a small scale combined heat and power plant
Carbon dioxide to air	1.1E+00	kg	Emissions profile based on a small scale combined heat and power plant
Methane to air	8.1E-04	kg	Emissions profile based on a small scale combined heat and power plant
Non-methane volatile organic compounds to air	9.5E-05	kg	Emissions profile based on a small scale combined heat and power plant
Dinitrogen monoxide to air	4.7E-05	kg	Emissions profile based on a small scale combined heat and power plant
Particulates, < 2.5 μm to air	2.9E-06	kg	Emissions profile based on a small scale combined heat and power plant
Heat, waste	1.6E+01	MJ	Emissions profile based on a small scale combined heat and power plant
Helium to air	2.3E-02	kg	Helium from
Heat, waste	9.4E+01	MJ	From electricity input
Disposal, polypropylene, 15.9% water, to municipal incineration/CH U	5.4E-01	kg	Disposal of the bucket
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	1.0E-02	kg	1% of total MWCNT production is assumed to be lost and sent to hazardous incinerator.
Treatment, sewage, to wastewater treatment, class 3/CH U	5.0E-03	m3	Waste water from cleaning the devices

- Infrastructure with respect to a chemical plant was accounted for using an existing dataset from the ecoinvent database[4]. The datasets considers the building and equipment for a chemical lab. In this report an input of 4 * 10-10 units of 'chemical plant, organics' per kg of produced material is suggested.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended in the ecoinvent report "Overview and Methodology"[5].
- Electricity is balanced with a European electricity mix[6].

Unit process: MWCNT, acid treated

In the acid treatment of MWCNT the catalyst used for the production of MWCNT (iron oxide, aluminium oxide) is removed. The MWCNT are resolved in nitric acid to remove the catalyst. The solution is filtered with a nylon membrane and dried. The acid is neutralised using sodium hydroxide and the resulting solution can be released to a WWT plant. As a precautionary measure, the MWCNT contaminated membrane is considered to be hazardous waste and sent to hazardous incineration plant. According to Professor Neophytides up scaling on industrial techniques allows a recycling rate of 90% for nitric acid[7]. The amount if recycled nitric acid is directly deducted from the input. Table S2 presents the LCI for the acid treatment of raw MWCNT.

Table S2. LCI for the production process of acid treated multiwalled carbon nanotubes (MWCNT).

Production of acid treated MWCNT			
Imputs	**Amount**	**unit**	**Remark**
MWCNT, at plant	1.0E+00	kg	Amount (1.04 kg) required to get 1.0 kg final MWCNT acid treated
Nitric acid, 50% in H2O, at plant/RER U	1.3E-01	kg	Agent to remove the electrocatalyst, value from Nanothinx
Sodium hydroxide, 50% in H2O, production mix, at plant/RER U	1.1E-01	kg	For the neutralisation of nitric acid, calculated based on stoichiometry
Nylon 66, at plant/RER U	3.1E-04	kg	Membrane for filtration process
Extrusion, plastic film/RER U	3.0E-03	kg	Extrusion process for the filter membrane
Water, ultrapure, at plant/GLO U	1.7E+00	kg	For cleaning of the devices, estimate Nanothinx
Soap, at plant/RER U	1.7E-03	kg	For cleaning of the devices
Electricity, low voltage, production RER, at grid/RER U	2.3E+00	kWh	Estimation nanothinx
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	7.7E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.3E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
MWCNT, acid treatment, at plant	1.0E+00	kg	Final product
Nitrate to air	3.9E-02	kg	From degradation of nitric acid
Heat, waste	8.4E+00	MJ	From electricity input
Treatment, sewage, to wastewater treatment, class 3/CH S	1.8E-03	m3	Disposal of the neuralised solution of nitric acid, sodium hydroxide, water, soap and the aluminium and iron oxide (3%)
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	1.9E-02	kg	Disposal of the membrane from filtration contaminated with 1% MWCNT

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with a chemical plant taken from the ecoinvent database.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Unit process: MWCNT Functionalisation

Functionalization is employed to achieve a desired surface property. For this the MWCNT are dissolved in organic solvents (Isoamyl nitrate, dimethylformamide). Then aminopyridine is added which attaches to the MWCNT. After this reaction the functionalised MWCNT are filtered and dried. The nylon membrane is contaminated with MWCNT and as a precautionary measure sent to hazardous incineration together with the potentially as well contaminated organic solvents. According to Professor Neophytides up scaling to industrial technique allows a recycling rate of 80% for the solvents[7]. The amount of recycled solvents is directly deducted from the input. Table S3 presents the LCI for the functionalised MWCNT.

Table S3. LCI for the production process of functionalised multiwalled carbon nanotubes (MWCNT).

Production of functionalised MWCNT			
Imputs	**Amount**	**unit**	**Remark**
MWCNT, acid treatment, at plant_v2	1.0E+00	kg	Amount (1.01 kg) required to get 1.0 kg final MWCNT functionalised
Solvents, organic, unspecified, at plant/GLO U	1.2E-01	kg	Two solvents are used: isoamyl nitrite and dimethylformamide. "Solvents, organics, unspecified" is used as proxy for isoamyl nitrite. Values from Nanothinx
N,N-dimethylformamide, at plant/RER U	6.6E-02	kg	
Pyridine-compounds, at regional storehouse/RER U	8.7E-01	kg	Proxy for aminopyridine, value from Nanothinx
Nylon 66, at plant/RER U	3.1E-04	kg	Membrane for filtration process
Extrusion, plastic film/RER U	3.0E-04	kg	Extrusion process for the filter membrane
Water, ultrapure, at plant/GLO U	1.7E+00	kg	For cleaning of the devices, estimate Nanothinx
Soap, at plant/RER U	1.7E-03	kg	For cleaning of the devices
Electricity, low voltage, production RER, at grid/RER U	2.3E+00	kWh	Estimation nanothinx
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	1.0E+00	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.7E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
MWCNT, functionalization, at plant	1.0E+00	kg	Final product
Heat, waste	8.4E+00	MJ	From electricity input
Organic substances to air	1.2E-02	kg	Evaporation of organic substances, value is assumption
Disposal, solvents mixture, 16.5% water, to hazardous waste incineration/CH U	1.3E-01	kg	Disposal of the solvents contaminated with MWCNT
Treatment, sewage, to wastewater treatment, class 3/CH S	1.7E-03	m3	Disposal of the water and soap
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	8.7E-01	kg	Disposal of the membrane from filtration contaminated with 1% MWCNT

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Electrocatalyst powder - Product specification

MWCNT are attractive candidates for a carbon support in PEM fuel cell applications due to the high specific surface area and unique electrical, mechanical and thermal properties. Moreover, CNTs have shown to be more corrosion resistant than carbon black under simulated fuel cell operation conditions. The unique characteristics of MWCNT allow reducing the platinum content in the electrocatalyst compared to carbon black used as support for the metal. The importance of the support material for platinum has been described by Orfanidi et al.[8]: "Decreasing the Pt loading especially at the cathodic electrodes can be pursued by optimizing the electrode structure in order to approach kinetically predicted voltage losses. Towards the development of an optimized electrocatalytic system, there are two important considerations: the deposition of platinum nanoparticles on the carbon support and the construction of the electrocatalytic layer so that they can thoroughly participate in the electrocatalytic active network of a 3D structured electrochemical interface, thus aiming to the total electrochemical utilization of Pt particles' specific surface area."

The platinum concentration for MWCNT and CB based electrocatalyst powder is 30%. The platinum nanoparticles are not produced in a separate step but rather simultaneously to the production of the electrocatalyst powder (Figure 2).

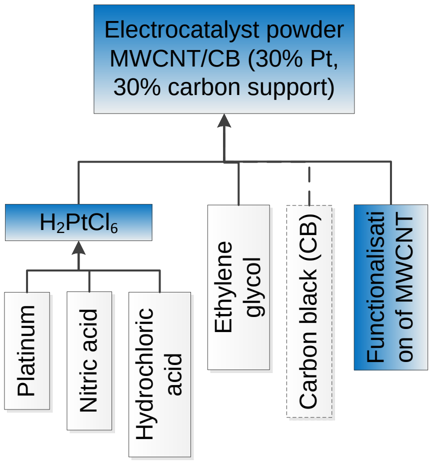


Figure S2. Product system overview for the production of electrocatalyst powder with either multiwalled carbon nanotubes (MWCNT) or carbon black (CB) as platinum support. Blue boxes refer to unit processes developed for this case study, white boxes are taken unaltered from ecoinvent.

Unit process: Hexachloroplatinic acid (H_2PtCl_6)

H_2PtCl_6 is the most readily available soluble compounds of platinum. H_2PtCl_6 is produced by dissolving platinum metal in aqua regia. Aqua regia or nitro-hydrochloric acid is a highly corrosive mixture of acids, a fuming yellow or red solution. The mixture is formed by freshly mixing concentrated nitric acid and hydrochloric acid. The process is taken from a patent[9], but the amount of acids are based on stoichiometric consideration. It is assumed that no losses of platinum will occur.

$$\mathrm{Pt} + 4\,\mathrm{HNO_3} + 6\,\mathrm{HCl} \rightarrow \mathrm{H_2PtCl_6} + 4\,\mathrm{NO_2} + 4\,\mathrm{H_2O}$$

Commercial platinum dissolved completely in a mixture of HCl and HNO_3 at a temperature at the boiling point of the nitric acid 86°C. Table S4 presents the LCI data for H_2PtCl_6.

Table S4. LCI for the production process of Hexachloroplatinic acid (H_2PtCl_6).

Production of Hexachloroplatinic acid			
Imputs	**Amount**	**unit**	**Remark**
Nitric acid, 50% in H2O, at plant/RER U	1.2E+00	kg	Values according to stoichiometry
Hydrochloric acid, 30% in H2O, at plant/RER U	1.8E+00	kg	Values according to stoichiometry
Platinum, primary, at refinery/ZA U	3.7E-01	kg	Values according to stoichiometry, 74.2% of platinum stems from South Africa
Platinum, primary, at refinery/RU U	1.0E-01	kg	Values according to stoichiometry, 20.7% of platinum stems from South Africa
Electricity, low voltage, production RER, at grid/RER U	1.8E-01	kWh	Accounts for the energy required heating up the solution.
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	1.1E+00	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	3.5E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
Hexachloroplatinic acid, at plant	1.0E+00	kg	Final product
Nitrogen oxides to air	4.5E-01	kg	Values according to stoichiometry
Heat, waste	6.6E-01	MJ	From electricity input
Treatment, sewage, to wastewater treatment, class 3/CH U	2.0E-03	m^3	water from chemical reactions, values according to stoichiometry

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Unit process: Electrocatalyst powder, MWCNT and CB

The dataset contains the production of an electrocatlayst for a PEM FC with platinum nanoparticles (~3 nm) as catalytic active metal. The amount of the platinum was calculated in order to obtain a final 30 wt.-% Pt in the final powder. Thus, the carbon support (MWCNT or CB) has a mass share of 70 wt.-%.

The MWCNT/CB is dispersed in ethylene glycol. Then the platinum precursor (H2PtCl6) is added. The solution is stirred for 12 hours at room temperature and the filtered, washed and dried. The data rely on industrial values, on literature and on stoichiometric considerations. Tables S5 and S6 present the LCI for both types of electrocatalyst powder.

Table S5. LCI for the production process of an electrocatalyst powder with multiwalled carbon nanotubes (MWCNT) as carbon support.

Production of Electrocatalyst powder, MWCNT			
Imputs	**Amount**	**unit**	**Remark**
MWCNT, functionalization, at plant	7.1E-01	kg	70% MWCNT in the final product
Ethylene glycol, at plant/RER U	6.7E-02	kg	Used as solvent for MWCNT
Hexachloroplatinic acid, at plant	6.4E-01	kg	Platinum precursor, value calculated so that the final share of Pt is 30 wt.%.
Nylon 66, at plant/RER U	3.1E-04	kg	Membrane for filtration process
Extrusion, plastic film/RER U	3.0E-04	kg	Extrusion process for the filter membrane
Water, ultrapure, at plant/GLO U	1.7E+00	kg	For cleaning of the devices, estimate Nanothinx
Soap, at plant/RER U	1.7E-03	kg	For cleaning of the devices
Electricity, low voltage, production RER, at grid/RER U	2.3E+00	kWh	Estimation Nanothinx
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	8.6E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.4E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
Electrocatalyst powder, MWCNT, at plant	1.0E+00	kg	Final product
Heat, waste	8.4E+00	MJ	From electricity input
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	1.4E-02	kg	Disposal of the membrane from filtration contaminated with 1% MWCNT
Treatment, sewage, to wastewater treatment, class 3/CH U	2.1E-03	m^3	Ethylene glycol and waste from the hexachloroplatinic acid

Table S6. LCI for the production process of an electrocatalyst powder with carbon black (CB) as carbon support.

Production of Electrocatalyst powder, CB			
Imputs	**Amount**	**unit**	**Remark**
Carbon black, at plant	7.1E-01	kg	70% Carbon black in the final product
Ethylene glycol, at plant/RER U	6.7E-02	kg	Used as solvent for CB
Hexachloroplatinic acid, at plant	6.4E-01	kg	Platinum precursor, value calculated so that the final share of Pt is 30 wt.%.
Nylon 66, at plant/RER U	3.1E-04	kg	Membrane for filtration process
Extrusion, plastic film/RER U	3.0E-04	kg	Extrusion process for the filter membrane
Water, ultrapure, at plant/GLO U	1.7E+00	kg	For cleaning of the devices, estimate Nanothinx
Soap, at plant/RER U	1.7E-03	kg	For cleaning of the devices
Electricity, low voltage, production RER, at grid/RER U	2.3E+00	kWh	Estimation nanothinx
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	8.6E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.4E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
Electrocatalyst powder, CB, at plant	1.0E+00	kg	Final product
Heat, waste	8.4E+00	MJ	From electricity input
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	1.4E-02	kg	Disposal of the membrane from filtration contaminated with 1% CB
Treatment, sewage, to wastewater treatment, class 3/CH U	2.1E-03	m^3	Ethylene glycol and waste from the hexachloroplatinic acid

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.

- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Membrane electrode assembly (MEA) - Product specification

A membrane electrode assembly is an assembled structure of polymer electrolyte membranes (PEM), catalyst and gas diffusion layer (GDL). The PEM is sandwiched between two electrodes which have the catalyst embedded in them. The electrodes – anode and cathode - are electrically insulated from each other by the PEM. The PEM is a fluoropolymer (PFSA) proton permeable but electrical insulator barrier. The barrier allows the transport of the protons from the anode to the cathode through the membrane but forces the electrons to travel around a conductive path to the cathode. The gas diffusion layer is a coated carbon cloth that consists mainly of polytetrafluoroethylene and carbon.

The electrocytalyst powder is sprayed on the gas diffusion layer. The GDE is subsequently calendared on the membrane to form the MEA.

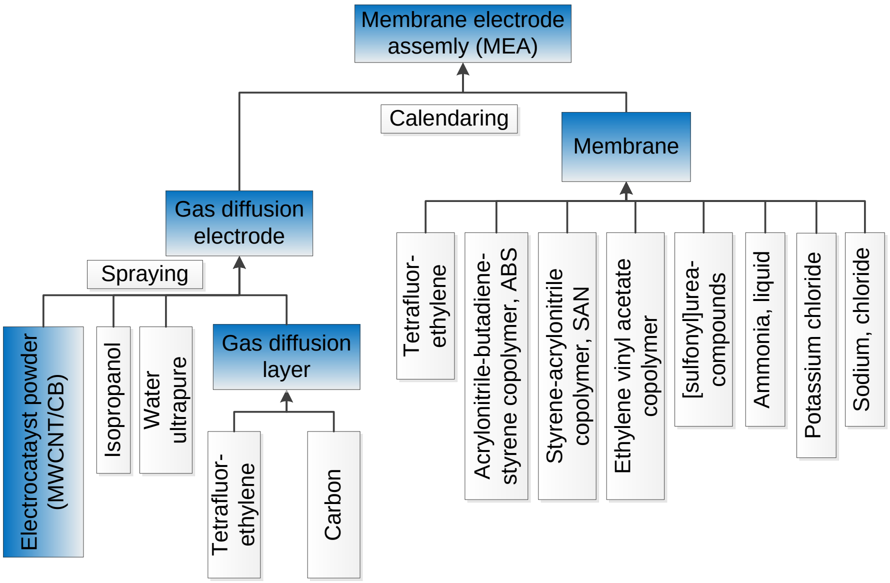


Figure S3. Product system overview for the production of a membrane electrode assembly with either MWCNT or CB as platinum support. Blue boxes refer to unit processes developed for this case study, white boxes are taken unaltered from ecoinvent.

Unit process: Gas diffusion electrode

The gas diffusion electrode (GDE) is the place where oxygen and fuel react at the gas diffusion electrodes, to form water, while converting the chemical bond energy into electrical energy. The gas diffusion electrode has to offer an optimal electric conductivity, in order to enable an electron transport with low ohmic resistance.

The GDE is a gas diffusion layer (GDL) coated with the electrocatalyst powder. The GDL consists of a polytetrafluoroethylene (15%) and carbon (85%). The electrocatalyst powder is applied on the GDL by a spraying and drying process. For that the electrocatalyst powder is solved in a solution of water and isopropanol[8]. Subsequently the GDE has to be dried. The data used for this process rely partly on industrial values (lab scale), on literature and on thermodynamic considerations (Tables S 7 and S8).

Table S7. LCI for the production process of a gas diffusion layer with multiwalled carbon nanotubes (MWCNT) as electrocatalyst powder.

Production of the gas diffusion electrode with MWCNT

Imputs	**Amount**	**unit**	**Remark**
Electrocatalyst powder, MWCNT, at plant	7.4E-04	kg	The platinum loading equals 2.2 mg/cm^2
Isopropanol, at plant/RER U	6.2E-01	kg	Solvent for the spraying process, ratio water solvent is 4:1
Water, ultrapure, at plant/GLO U	2.9E+00	kg	Solvent for the spraying process, ratio water solvent is 4:1, 1 kg water is used for cleaning purpose
Graphite, at plant/RER U	1.2E-03	kg	Proxy for the gas diffusion layer, Assumption: 85% of the mass is graphite, 15% is PTFE
Tetrafluoroethylene, at plant/RER U	2.1E-04	kg	
Electricity, low voltage, production RER, at grid/RER U	1.3E+00	kWh	Based on specific heat capacity and enthalpy of evaporation for the drying process
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	1.0E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.7E-02	tkm	Standard distances from ecoinvent guidelines
Outputs			
Gas diffusion electrode, MWCNT, at plant	1.0E+00	dm^2	Final product
Water to air	1.9E-03	m^3	Evaporating the solvent
2-Propanol	6.2E-01	kg	Evaporating the solvent
Heat, waste	4.7E+00	MJ	From electricity input
Treatment, sewage, to wastewater treatment, class 3/CH U	1.0E-03	m3	For cleaning of the devices
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	9.1E-06	kg	Gas diffusion layer scrap

Table S8. LCI for the production process of a gas diffusion layer with Carbon black (MWCNT) as electrocatalyst powder.

Production of the gas diffusion electrode with CB

Imputs	**Amount**	**unit**	**Remark**
Electrocatalyst powder, CB, at plant	1.0E-03	kg	The platinum loading equals 3 mg/cm^2
Isopropanol, at plant/RER U	8.4E-01	kg	Solvent for the spraying process, ratio water solvent is 4:1
Water, ultrapure, at plant/GLO U	3.5E+00	kg	Solvent for the spraying process, ratio water solvent is 4:1, 1 kg water is used for cleaning purpose
Graphite, at plant/RER U	1.2E-03	kg	Proxy for the gas diffusion layer, Assumption: 85% of the mass is graphite, 15% is PTFE
Tetrafluoroethylene, at plant/RER U	2.1E-04	kg	
Electricity, low voltage, production RER, at grid/RER U	1.8E+00	kWh	Based on specific heat capacity and enthalpy of evaporation for the drying process
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	1.5E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	2.5E-02	tkm	Standard distances from ecoinvent guidelines
Outputs			
Gas diffusion electrode, CB, at plant	1.0E+00	dm^2	Final product
Water to air	2.5E-03	m^3	Evaporating the solvent
2-Propanol	8.4E-01	kg	Evaporating the solvent
Heat, waste	6.5E+00	MJ	From electricity input
Treatment, sewage, to wastewater treatment, class 3/CH U	1.0E-03	m3	For cleaning of the devices
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	9.1E-06	kg	Gas diffusion layer scrap

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Unit process: Membrane

A PEM is a semipermeable membrane generally made from ionomers and designed to conduct protons while being impermeable to gases such as oxygen, hydrogen, natural gas, reformate etc. The essential function when incorporated into an MEA of a fuel cell is to separate reactants from the transport of protons. One of the most common and commercially available PEM materials is the fluoropolymer Nafion. Nafion is a sulfonated tetrafluoroethylene based fluoropolymer-copolymer, a synthetic polymer with ionic properties which are called ionomers. Nafion's unique ionic properties are a result of incorporating perfluorovinyl ether groups terminated with sulfonate groups onto a tetrafluoroethylene backbone [10, 11]. Nafion has received a considerable amount of attention as a proton conductor for proton exchange membrane (PEM) fuel cells because of its excellent thermal and mechanical stability.

Nafion derivatives are first synthesized by the copolymerization of tetrafluoroethylene and a derivative of a perfluoro (alkyl vinyl ether) with sulfonyl acid fluoride. The resulting product is a sulfonyl fluoride ($-SO_2F$) containing thermoplastic that is extruded into films. Hot aqueous NaOH converts these ($-SO_2F$) groups into sulfonate groups ($-SO_3{-}Na+$). This form of Nafion, referred to as the neutral or salt form, is finally converted to the acid form containing the sulfonic acid ($-SO_3H$) groups. Nafion can be cast into thin films by heating in aqueous alcohol at 250 °C in an autoclave. The life cycle inventory model (Table S9) follows mainly the originally developed process by Grot[12, 13].

Table S9. LCI for the production process of a polymer electrolyte membrane.

Production of a polymer electrlyte membrane (Nafion)			
Imputs	**Amount**	**unit**	**Remark**
Tetrafluoroethylene, at plant/RER U	9.3E-01	kg	copolymer tetrafluorethylene; mol-ratio copolymer 1:copolymer 2 equals 7.5:1
Acrylonitrile-butadiene-styrene copolymer, ABS, at plant/RER U	3.1E-02	kg	represents copolymer 2: 3,6-dioxa-4-methyl-7-octene sulfonyl fluoride with equal shares for each copolymer, mol-ratio copolymer 1:copolymer 2 equals 7.5:1
Styrene-acrylonitrile copolymer, SAN, at plant/RER U	3.1E-02	kg	
Ethylene vinyl acetate copolymer, at plant/RER U	3.1E-02	kg	
[sulfonyl]urea-compounds, at regional storehouse/RER U	3.1E-02	kg	
Calandering PVC foil B250	1.0E+00	kg	energy consumption included in the process
Ammonia, liquid, at regional storehouse/RER U	9.7E-01	kg	used to "boil" the copolymers, value is an estimate
Ammonia, liquid, at regional storehouse/RER U	9.3E-03	kg	represents the production of potassium amide
Potassium chloride, as K2O, at regional storehouse/RER U	4.1E-02	kg	
Sodium, chloride electrolysis	1.3E-02	kg	
Heat, unspecific, in chemical plant/RER U	3.0E-02	MJ	heat required for the production of potassium amid
Electricity, low voltage, production UCTE, at grid/UCTE U	1.1E+00	kWh	electricity required for the production of potassium amid
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	8.3E-01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	2.1E-01	tkm	Standard distances from ecoinvent guidelines
Outputs			
Polymer electrolyte membrane, at plant	1.0E+00	kg	Final product
Heat, waste	3.8E+00	MJ	From electricity input
Hydrogen	5.5E-04	kg	from the reaction of liquid ammonia with potassium chloride
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH S	3.2E-02	kg	NaCl from the production of potassium amide

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Unit process: Membrane electrode assembly

The unit process contains the calendaring of a GDL on a PEM to a MEA. The GDL is coated either with an electrocatalyst powder with MWCNT or CB as carbon support. The thickness of the PEM in the present application is assumed to be 50 μm[14]. Tables S10 and S11 provide the Life cycle inventory for the MEA with MWCNT and CB as carbon support for the electrocatalyst.

Table S10. LCI for the production process of a membrane electrode assembly (MEA) with multiwalled carbon nanotubes (MWCNT) as carbon support for the electrocatalyst.

Production of an MEA (MWCNT as carbon support)

Imputs	Amount	unit	Remark
Polymer electrolyte membrane, at plant	1.2E-03	kg	mass based on assumed thickness of 50 µm and a density equal to PTFE
Gas diffusion layer, MWCNT, at plant	1.0E+00	dm2	refers to the functional unit
Electricity, low voltage, production RER, at grid/RER U	1.7E-02	kWh	Calendaring of the MEA
Transport, freight, rail/RER U	6.9E-05	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.2E-05	tkm	Standard distances from ecoinvent guidelines
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Outputs			
MEA, MWCNT, at plant	1.0E+00	dm^2	Fianal product
Heat, waste	6.0E-02	MJ	From electricity input
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	5.5E-05	kg	membrane scrap

Table S11. LCI for the production process of a membrane electrode assembly (MEA) with carbon black (CB) as carbon support for the electrocatalyst.

Production of an MEA (CB as carbon support)

Imputs	Amount	unit	Remark
Polymer electrolyte membrane (Nafion), at plant	1.2E-03	kg	mass based on assumed thickness of 50 µm and a density equal to PTFE
Gas diffusion layer, CB, at plant	1.0E+00	dm2	refers to the functional unit
Electricity, low voltage, production RER, at grid/RER U	1.7E-02	kWh	Calendaring of the MEA
Transport, freight, rail/RER U	6.9E-05	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	1.2E-05	tkm	Standard distances from ecoinvent guidelines
Chemical plant, organics/RER/I U	4.0E-10	p	Standard from ecoinvent guidelines
Outputs			
MEA, CB, at plant	1.0E+00	dm^2	Fianal product
Heat, waste	6.0E-02	MJ	From electricity input
Disposal, hazardous waste, 25% water, to hazardous waste incineration/CH U	5.5E-05	kg	membrane scrap

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

PEM fuel cell unit - Product specification

Many of the MEAs are stacked between flow plates, in which each flow plate is sealed against the next one. The cell stack is sandwiched between end plates. The endplates are screwed together under moderated pressure on to the MEAs so that it is ensured that each MEA is sealed. The endplates are finally equipped with fittings for gas inlet and outlet. The cell stack is placed in a casing and equipped with a balance of plant (BoP). Figure S4 illustrates the product system for the PEM fuel cell unit.

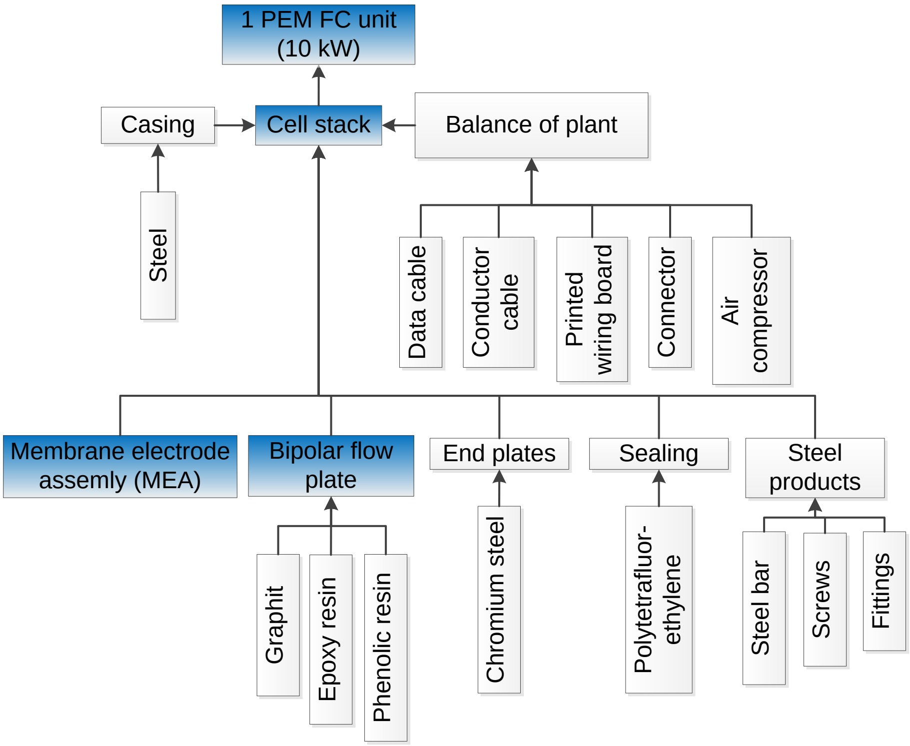


Figure S4. Product system overview for the production of a fuel cell unit. Blue boxes refer to unit processes developed for this case study, white boxes are taken unaltered from ecoinvent.

Unit process: Bipolar flow plates

The bipolar flow plate is a multi-functional component within a PEM fuel cell stack. Its primary function is to supply reactant gases to the GDL via flow channels. The effectiveness of reactant transport depends partially on the art of the flow-field design[15], so the alternative name for a bipolar plate is the flow-field plate. Bipolar flow plates must provide electrical connections between the individual cells. They have to remove the water produced at the cathode effectively. Bipolar plates must also be relatively impermeable to gases, sufficiently strong to withstand stack assembly and easily mass-produced. Production of the great majority of carbon-polymer composites involves the hot moulding of carbon or graphite filler in a thermosetting matrix (epoxy resin, phenolic resins). Typical carbon contents range between 50 and 80 % by weight. The Life cycle inventory data (Table S12) is mainly based on literature data[16, 17].

Table S12. LCI for the production process of a bipolar flow plate.

Production of bipolar flowplate			
Imputs	**Amount**	**unit**	**Remark**
Graphite, at plant/RER U	2.7E-02	kg	65% Graphite
Phenolic resin, at plant/RER U	7.2E-03	kg	Assumption: Equal shares for phenolic and epoxy resin (17.5%)
Epoxy resin, liquid, at plant/RER U	7.2E-03	kg	
Electricity, low voltage, production RER, at grid/RER U	1.1E-03	kWh	For the hot molding process
Metal working factory operation, average heat energy/RER U	1.3E-14	kg	Standard from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	2.9E-03	tkm	Standard distances from ecoinvent guidelines
Transport, freight, rail/RER U	1.3E-02	tkm	Standard distances from ecoinvent guidelines
Outputs			
Bipolar flowplate, at plant	1.0E+00	dm^2	Final product
Heat, waste	4.1E-03	MJ	From electricity input
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	2.1E-03	kg	5% scrap

- Electricity is balanced with a European electricity mix.
- Infrastructure is represented with the chemical plant from ecoinvent.
- Road and rail transport is taken into account using standard distances for the European geographical situation as recommended from ecoinvent.

Unit process: Cell stack

The cell stack assembly is a process where numerous MEAs are stacked, each one separated by a bipolar flow plate. The number of single MEA included in the cell stack determines the peak power of the fuel cell. Each bipolar flow plate is sealed against the next one with PTFE preventing a bypass of reactants (fuel and air) to the wrong side of the electrode. The cell stack is sandwiched between endplates and fixed with screws with moderate pressure so that electric conductivity is assured. The endplates are equipped with fittings for fuel inflow and water vapour outlet. The LCI data for the cell stacks with MWCNT and CB are shown in Table S13 and Table S14.

Table S13. LCI for the production process of a 10 kW PEM fuel cell stack with multiwalled carbon nanotubes (MWCNT).

Production of a 10 kW PEMFC Stack (MWCNT)			
Imputs	**Amount**	**unit**	**Remark**
MEA, MWCNT, at plant	7.7E+02	dm2	
Bipolar flowplate, at plant	9.7E+02	dm2	
Chromium steel 18/8, at plant/RER U	9.9E+00	kg	Endplate
Steel product manufacturing, average metal working/RER U	1.5E+00	kg	Refers to steel bars and screws to fix the stack and to fittings
Tetrafluoroethylene, at plant/RER U	1.5E+00	kg	Sealing of bipolar flowplates
Metal working factory/RER/I U	3.5E-09	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	3.1E+01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	5.1E+00	tkm	Standard distances from ecoinvent guidelines
Outputs			
PEM Fuel cell stack, MWCNT, 10 kW, at plant	1.0E+00	unit	Final product

Table S14. LCI for the production process of a 10 kW PEM fuel cell stack with carbon black (CB).

Production of a 10 kW PEMFC Stack (CB)			
Imputs	**Amount**	**unit**	**Remark**
MEA, CB, at plant	7.7E+02	dm2	
Bipolar flowplate, at plant	9.7E+02	dm2	
Chromium steel 18/8, at plant/RER U	9.9E+00	kg	Endplate
Steel product manufacturing, average metal working/RER U	1.5E+00	kg	Refers to steel bars and screws to fix the stack and to fittings
Tetrafluoroethylene, at plant/RER U	1.5E+00	kg	Sealing of bipolar flowplates
Metal working factory/RER/I U	3.5E-09	p	Standard from ecoinvent guidelines
Transport, freight, rail/RER U	3.1E+01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	5.1E+00	tkm	Standard distances from ecoinvent guidelines
Outputs			
PEM Fuel cell stack, CB, 10 kW, at plant	1.0E+00	unit	Final product

Unit process: Fuel cell unit

The PEM fuel cell stack is placed in a casing and equipped with the balance of plant (BoP). For combined heat and power the PEM fuel cell is typically stored in a steel box together with other equipment required for a combined heat and power plant. The steel sheet is assumed to have the dimension of the PEM FC plus 2 cm space to each side and a thickness of 1 mm.

The balance of plant is the infrastructure of a fuel cell, not including the single cells. Electrical and mechanical infrastructure is required, such as cables, printed wiring boards, clamp connector and connectors for electronic devices or a gas compressor. The gas compressor has to produce a specific pressure on the fuel to be fed efficiently into the fuel cells. The LCI data for the production of a PEM fuel cell is provided in Table S15 and S16.

Table S15. LCI for the production process of a 10 kW PEM fuel cell unit with multiwalled carbon nanotubes (MWCNT).

Production of a 10 kW PEMFC (MWCNT)			
Imputs	**Amount**	**unit**	**Remark**
PEM Fuel cell stack, MWCNT, 10 kW, at plant	1.0E+00	unit	
Printed wiring board, surface mounted, unspec., solder mix, at plant/GLO U	6.5E-02	kg	Assumed the same amount as a li-ion battery
Air compressor, screw-type compressor, 4 kW, at plant/RER/I U	1.0E-01	p	Assumption: 10% is sufficient in order to provide enough pressure to feed the fuel cell with fuel
Cable, data cable in infrastructure, at plant/GLO U	5.0E+00	m	Assumed the same amount as a li-ion battery
Cable, three-conductor cable, at plant/GLO U	5.0E-01	m	Assumed the same amount as a li-ion battery
Sheet rolling, steel/RER U	6.3E+00	kg	Casing: dimension: 3.4x3.4x4.2 dm; thickness of the sheet 1 mm
Steel, converter, unalloyed, at plant/RER U	6.3E+00	kg	Casing: dimension: 3.4x3.4x4.2 dm; thickness of the sheet 1 mm
Connector, clamp connection, at plant/GLO U	2.0E-02	kg	Assumption
Connector, computer, peripherical type, at plant/GLO U	2.0E-02	kg	Assumption
Connector, PCI bus, at plant/GLO U	2.0E-02	kg	Assumption
Transport, freight, rail/RER U	4.4E+01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	7.3E+00	tkm	Standard distances from ecoinvent guidelines
Outputs			
PEM Fuel cell, MWCNT, 10 kW, at plant	1.0E+00	unit	Final product

Table S16. LCI for the production process of a 10 kW PEM fuel cell unit with carbon black (CB).

Production of a 10 kW PEMFC (CB)			
Imputs	**Amount**	**unit**	**Remark**
PEM Fuel cell stack, CB, 10 kW, at plant	1.0E+00	unit	
Printed wiring board, surface mounted, unspec., solder mix, at plant/GLO U	6.5E-02	kg	Assumed the same amount as a li-ion battery
Air compressor, screw-type compressor, 4 kW, at plant/RER/I U	1.0E-01	p	Assumption: 10% is sufficient in order to provide enough pressure to feed the fuel cell with fuel
Cable, data cable in infrastructure, at plant/GLO U	5.0E+00	m	Assumed the same amount as a li-ion battery
Cable, three-conductor cable, at plant/GLO U	5.0E-01	m	Assumed the same amount as a li-ion battery
Sheet rolling, steel/RER U	6.3E+00	kg	Casing: dimension: 3.4x3.4x4.2 dm; thickness of the sheet 1 mm
Steel, converter, unalloyed, at plant/RER U	6.3E+00	kg	Casing: dimension: 3.4x3.4x4.2 dm; thickness of the sheet 1 mm
Connector, clamp connection, at plant/GLO U	2.0E-02	kg	Assumption
Connector, computer, peripherical type, at plant/GLO U	2.0E-02	kg	Assumption
Connector, PCI bus, at plant/GLO U	2.0E-02	kg	Assumption
Transport, freight, rail/RER U	4.4E+01	tkm	Standard distances from ecoinvent guidelines
Transport, lorry >16t, fleet average/RER U	7.3E+00	tkm	Standard distances from ecoinvent guidelines
Outputs			
PEM Fuel cell, MWCNT, 10 kW, at plant	1.0E+00	unit	Final product

Disposal of a PEM fuel cell – Product system.

Most components of a PEM fuel cell have considerable value so that it is worth to recycle the materials. The benefit of recycling is accounted for using an "avoided burden" model[5]. This approach calculates the difference between the environmental burdens of the recycling process and those of the disposal and standard production of the corresponding good. An overview of disposed components is shown in Figure S5.

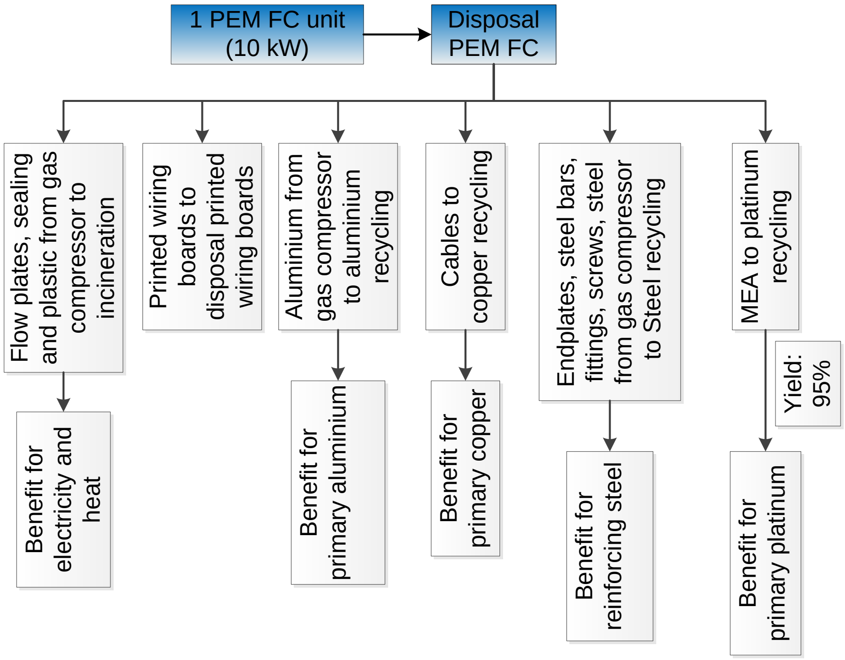


Figure S5. Disposal model for a fuel cell unit at its end of life. Blue boxes refer to unit processes developed for this case study, white boxes are taken unaltered from ecoinvent.

Unit process: Disposal PEM FC

The avoided burden approach shall be explained base on 2 examples:

1. The MEA of the PEM fuel cell is sent to recycling. The model accounts for all environmental impacts due to 100% of the platinum content sent to the recycling process. Platinum is recycled with a recycling rate of 95% [79]. The recycled platinum substitutes virgin platinum. For that reason there is a benefit given that neutralises the impacts originally balanced in the amount of 95% of virgin platinum.

2. Some components may not be recycled but rather sent to incineration (sealing material, flowplates, plastic). In an incineration plant the materials contribute to the production of electricity and heat. For these materials the environmental burdens of the incineration process are balanced. In contrast, the model benefits for the amount of electricity (European electricity mix) and heat (from natural gas) substituted.

The resulting LCI using the avoided burden approach is presented in Table S17 (MWCNT) and S18 (CB).

Table S17. LCI for the disposal of a PEM fuel cell with multiwalled carbon nanotubes (MWCNT) using an avoided burden approach.

Disposal of a 10 kW PEM FC (MWCNT)			
Imputs	**Amount**	**unit**	**Remark**
Platinum, secondary, at refinery/RER U	1.7E-01	kg	Pt in MEA to precius metal recycling
Platinum, primary, at refinery/ZA U	-1.3E-01	kg	0.159 kg Pt in 2.30 kg MEA, Pt recycling rate assumed to be 95%, Benefit for primary Russian production (78.2% share)
Platinum, primary, at refinery/RU U	-3.5E-02	kg	0.159 kg Pt in 2.30 kg MEA, Pt recycling rate assumed to be 95%, Benefit for primary Russian production (21.8% share)
Copper, secondary, at refinery/RER U	2.3E+00	kg	5 m data cable with 0.0156 kg Cu/m, 0.5 m 3 phse conductor cable 0.492 kg Cu/m, 2 kg copper from gas compressor
Copper, at regional storage/RER U	-1.9E+00	kg	Benfit for copper recycling, recycling rate assumed to be 80%
Electricity, low voltage, production UCTE, at grid/UCTE U	-4.3E+01	MJ	Benefit for the disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor, substituting electricity (1.01 MJ/kg)
Heat, natural gas, at boiler atm. low-NOx condensing non-modulating <100kW/RER U	-9.3E+01	MJ	Benefit for the disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor, substituting heat (2.16MJ/kg)
Iron scrap, at plant/RER U	2.6E+01	kg	Endplates, steel bars, screws, fittings, casing, connector and steel products form gas compressor to recycling
Pig iron, at plant/GLO U	-2.1E+01	kg	Benefit for steel recycling, recycling rate assumed to be 80%
Aluminium, secondary, from old scrap, at plant/RER S	2.0E+00	kg	Aluminium from gas compressor to recycling
Aluminium, primary, at plant/RER U	1.6E+00	kg	Benefit for aluminium recycling, recycling rate assumed to be 80%
Outputs			
Disposal, PEM fuel cell (MWCNT), 10 kW	1.0E+00	unit	
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	4.3E+01	kg	disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor,
Disposal, treatment of printed wiring boards/GLO U	1.5E-01	kg	Disposal PWB from fuel cell and gas compressor

Table S18. LCI for the disposal of a PEM fuel cell with carbon black (CB) using an avoided burden approach.

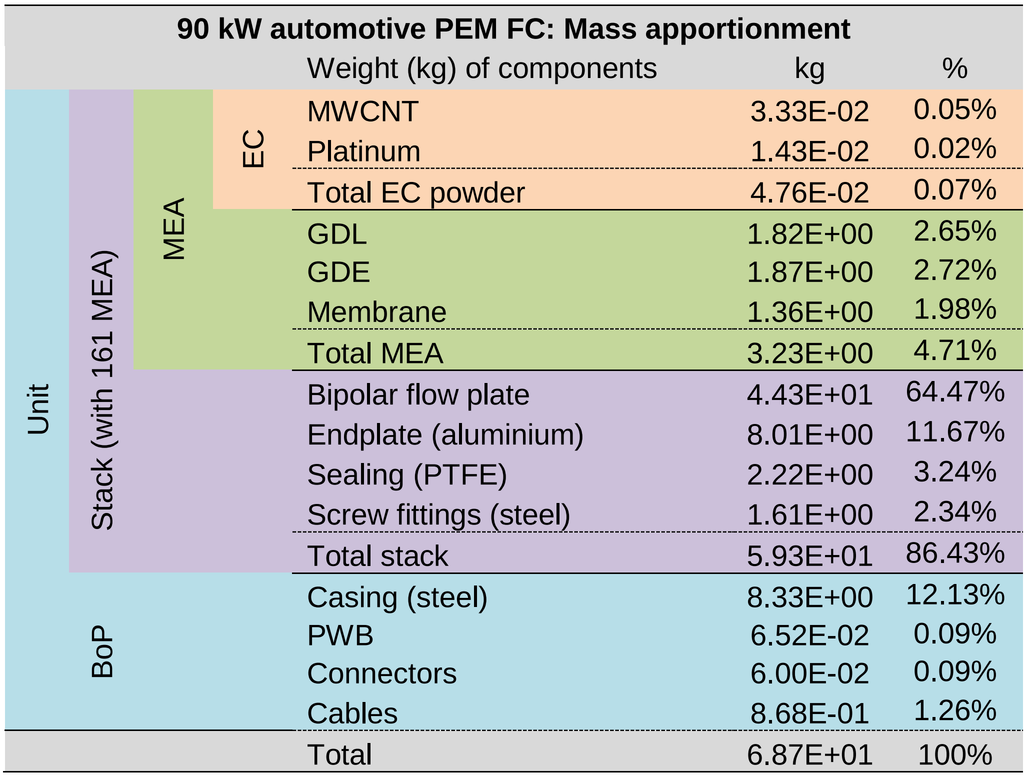
Disposal of a 10 kW PEM FC (CB)

Imputs	**Amount**	**unit**	**Remark**
Platinum, secondary, at refinery/RER U	2.3E-01	kg	Pt in MEA to precius metal recycling
Platinum, primary, at refinery/ZA U	-1.7E-01	kg	0.159 kg Pt in 2.30 kg MEA, Pt recycling rate assumed to be 95%, Benefit for primary Russian production (78.2% share)
Platinum, primary, at refinery/RU U	-4.8E-02	kg	0.159 kg Pt in 2.30 kg MEA, Pt recycling rate assumed to be 95%, Benefit for primary Russian production (21.8% share)
Copper, secondary, at refinery/RER U	2.3E+00	kg	5 m data cable with 0.0156 kg Cu/m, 0.5 m 3 phse conductor cable 0.492 kg Cu/m, 2 kg copper from gas compressor
Copper, at regional storage/RER U	-1.9E+00	kg	Benfit for copper recycling, recycling rate assumed to be 80%
Electricity, low voltage, production UCTE, at grid/UCTE U	-4.3E+01	MJ	Benefit for the disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor, substituting electricity (1.01 MJ/kg)
Heat, natural gas, at boiler atm. low-NOx condensing non-modulating <100kW/RER U	-9.3E+01	MJ	Benefit for the disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor, substituting heat (2.16MJ/kg)
Iron scrap, at plant/RER U	2.6E+01	kg	Endplates, steel bars, screws, fittings, casing, connector and steel products form gas compressor to recycling
Pig iron, at plant/GLO U	-2.1E+01	kg	Benefit for steel recycling, recycling rate assumed to be 80%
Aluminium, secondary, from old scrap, at plant/RER S	2.0E+00	kg	Aluminium from gas compressor to recycling
Aluminium, primary, at plant/RER U	1.6E+00	kg	Benefit for aluminium recycling, recycling rate assumed to be 80%
Outputs			
Disposal, PEM fuel cell (CB), 10 kW	1.0E+00	unit	
Disposal, municipal solid waste, 22.9% water, to municipal incineration/CH U	4.3E+01	kg	disposal of the bipolar flow plates, PTFE from sealing, plastic from air compressor,
Disposal, treatment of printed wiring boards/GLO U	1.5E-01	kg	Disposal PWB from fuel cell and gas compressor

Table S19. Mass apportionment for a 1 kW HT PEM FC for micro combined heat and power. MEA: membrane electrode assembly; MWCNT: Multiwalled carbon nanotubes; CB: Carbon black; EC: Electrocatalyst; GDL: Gas diffusion layer; PTFE: Polytetrafluoroethylene; PWB: Printed wiring board; BoP: Balance of plant.

1 kW HT PEM FC for μ-CHP - Mass apportionment						
				Weight (kg) of components	kg	%
Unit	Stack (with 19 MEA)	MEA	EC	MWCNT	3.99E-02	0.20%
				Platinum	1.71E-02	0.09%
				Total electrocatalyst powder	5.70E-02	0.29%
				Carbon cloth	1.09E-01	0.56%
				Coated carbon cloth (GDL)	1.66E-01	0.85%
				Membrane	8.15E-02	0.42%
				Total MEA	2.47E-01	1.26%
				Bipolar flow plate	4.05E+00	20.67%
				Endplate (stainless steel)	4.52E+00	23.07%
				Sealing (PTFE)	1.72E-01	0.88%
				Screw fittings (steel)	6.13E-01	3.13%
				Total stack	9.60E+00	49.00%
	BoP			Casing (steel)	2.01E+00	10.26%
				PWB	6.52E-02	0.33%
				Connectors	6.00E-02	0.31%
				Cables	8.68E-01	4.43%
				Air compressor	6.99E+00	35.67%
				Total unit	1.96E+01	100%

Table S20. Mass apportionment for a 90 kW PEM FC for automotive application. MEA: membrane electrode assembly; MWCNT: Multiwalled carbon nanotubes; CB: EC: Electrocatalyst; GDL: Gas diffusion layer; GDE: Gas diffusion electrode; PTFE: Polytetrafluoroethylene; PWB: Printed wiring board; BoP: Balance of plant.



90 kW automotive PEM FC: Mass apportionment

				Weight (kg) of components	kg	%
Unit	Stack (with 161 MEA)	MEA	EC	MWCNT	3.33E-02	0.05%
				Platinum	1.43E-02	0.02%
				Total EC powder	4.76E-02	0.07%
				GDL	1.82E+00	2.65%
				GDE	1.87E+00	2.72%
				Membrane	1.36E+00	1.98%
				Total MEA	3.23E+00	4.71%
				Bipolar flow plate	4.43E+01	64.47%
				Endplate (aluminium)	8.01E+00	11.67%
				Sealing (PTFE)	2.22E+00	3.24%
				Screw fittings (steel)	1.61E+00	2.34%
				Total stack	5.93E+01	86.43%
	BoP			Casing (steel)	8.33E+00	12.13%
				PWB	6.52E-02	0.09%
				Connectors	6.00E-02	0.09%
				Cables	8.68E-01	1.26%
				Total	6.87E+01	100%

Table S21. Mass and environmental impacts in ReCiPe for the basic components of a 10 kW HTPEM FC with multiwalled carbon nanotubes as carbon substrate.

Component	Mass (kg)	Mass (%)	ReCiPe (points)	ReCiPe (%)
MWCNT	0.40	0.5%	1.4	0.1%
Platinum	0.17	0.2%	2470.5	89.4%
Carbon cloth	1.1	1.4%	21.7	0.8%
Polymer electrolyte membrane	0.81	1.1%	13.7	0.5%
Spraying process (Isopropanol)	0.0	0.0	116	4.2%
Membrane electrode assembly	2.7	3.5%	2698.3	97.6%
Bipolar flow plates	40.2	52.2%	8.9	0.3%
Sealing of bipolar flow plates	1.5	1.9%	23.6	0.9%
Endplates	9.9	12.8%	11.2	0.4%
Fuel cell stack	55.8	72.4%	2742.5	99.2%
Balance of plant	21.3	27.6%	22.0	0.8%
Fuel cell unit	77.1	100.0%	2764.5	100.0%

Table S22. Numerical values for midpoint, endpoint and single score indicators of production, disposal and overall environmental impacts for both types of HT PEM fuel cells in ReCiPe point.

		Production		End of life		Overall	
midpoint	endpoint	CB	MWCNT	CB	MWCNT	CB	MWCNT
Climate change Human Health	Damage to Human health	187	145	-91.4	-67.0	95.1	78.3
Ozone depletion	Damage to Human health	1.43	1.43	-0.01	-0.01	1.42	1.42
Human toxicity	Damage to Human health	365	270	-326	-239	38	31
Photochemical oxidant formation	Damage to Human health	0.22	0.16	-0.05	-0.04	0.17	0.12
Particulate matter formation	Damage to Human health	794	584	-734	-536	60	48
Ionising radiation	Damage to Human health	0.90	0.67	-0.58	-0.43	0.32	0.24
	Total: Damage to Human health	1348	1002	-1153	-842	195	160
Climate change Ecosystems	Damage to Ecosystem Quality	118	92	-58	-42	60	50
Terrestrial acidification	Damage to Ecosystem Quality	9.03	6.64	-8.42	-6.15	0.61	0.49
Freshwater eutrophication	Damage to Ecosystem Quality	1.62	1.20	-1.40	-1.03	0.22	0.18
Terrestrial ecotoxicity	Damage to Ecosystem Quality	0.13	0.10	-0.09	-0.06	0.04	0.04
Freshwater ecotoxicity	Damage to Ecosystem Quality	1.29	0.96	-1.15	-0.84	0.14	0.12
Marine ecotoxicity	Damage to Ecosystem Quality	0.24	0.18	-0.22	-0.16	0.03	0.02
Agricultural land occupation	Damage to Ecosystem Quality	3.70	2.88	-2.30	-1.69	1.40	1.19
Urban land occupation	Damage to Ecosystem Quality	3.73	2.81	-3.04	-2.23	0.69	0.58
Natural land transformation	Damage to Ecosystem Quality	3.67	2.75	-2.68	-1.96	0.99	0.79
	Total: Damage to Ecosystem Quality	141	109	-77	-57	64	53
Metal depletion	Damage to Resource Quality	2004	1475	-1874	-1368	130	106
Fossil depletion	Damage to Resource Quality	239	178	-102	-75	136	103
	Total: Damage to Resource Quality	2242	1653	-1976	-1443	266	210
	Single score (Total)	3731	2765	-3206	-2342	525	422

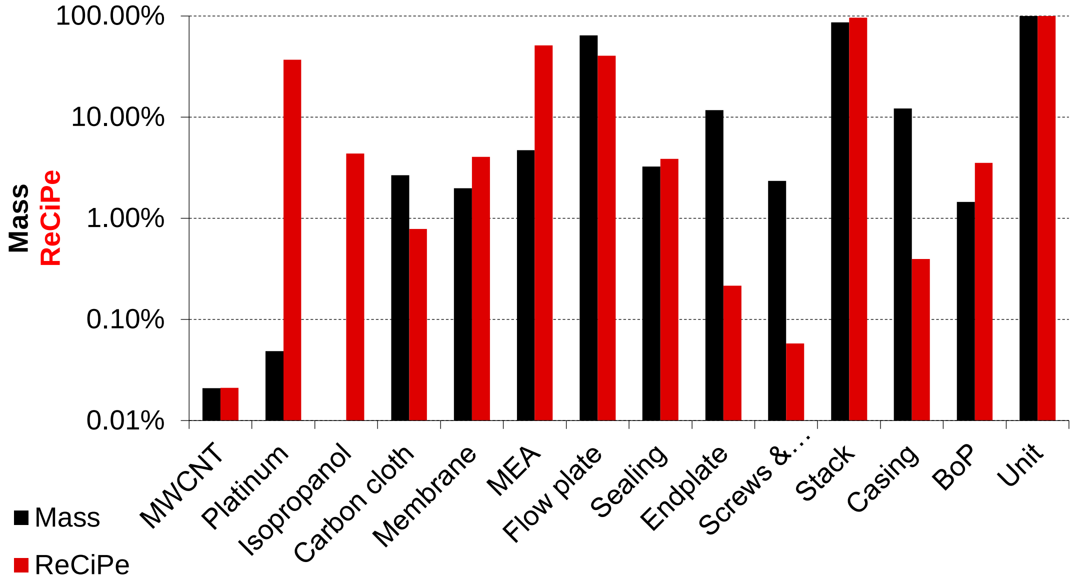


Figure S6. Mass (%; black bars) versus environmental impacts in ReCiPe (%; red bars) for the basic components of an automotive PEM FC on a log scale. MWCNT: multiwalled carbon nanotubes; MEA: membrane electrode assembly; BoP: balance of plant.

Table S23. Mass and environmental impacts in ReCiPe for the basic components of a 90 kW HTPEM FC with multiwalled carbon nanotubes as carbon substrate.

Component	ReCiPe (points)	ReCiPe (%)	Mass (kg)	Mass (%)
MWCNT	0.119	0.02%	0	0.021%
Platinum	209	36.8%	0	0.049%
Isopropanol	24.7	4.37%		
Carbon cloth	4.44	0.78%	2	2.65%
Membrane	23.0	4.06%	1	1.98%
MEA	291	51.4%	3	4.70%
Flow plate	229	40.5%	44	64.5%
Sealing	21.9	3.86%	2	3.24%
Endplate	1.22	0.22%	8	11.7%
Screws & fittings	0.328	0.06%	2	2.3%
Stack	544	96.0%	59	86.4%
Casing	2.23	0.39%	8	12.1%
BoP	20.0	3.54%	1	1.45%
Unit	566	100.00%	69	100.0%

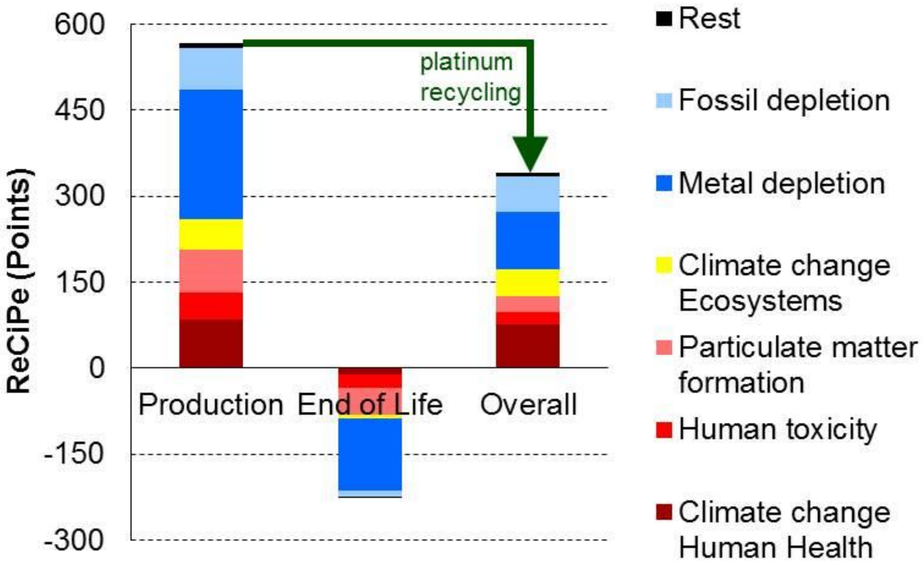


Figure S7. Production, end of life treatment and overall environmental performance for the automotive PEM fuel cells in ReCiPe point split into the three endpoints (reddish colours: damage to human health; yellow: damage to ecosystem; blueish colours: damage to resource depletion) and 6 midpoint indicators. “Rest” represents the remaining 11 midpoint indicators all together.

Table S24. Environmental burdens expressed as ReCiPe points, climate change impacts and energetic efficiency expressed as cumulated energy demand for a transport service of 1 km travelled by an ICEV (internal combustion engine vehicle), a BEV (battery electric vehicle) and a FCEV (fuel cell electric vehicle). P: production; M: maintenance: D: disposal; li-ion: lithium ion battery; PEM: polymer electrolyte membrane fuel cell.

	ReCiPe (millipoints/km)			Climate change (kgCO_2 eq./km)			Cumulated energy demand (MJ/km)		
	ICEV	BEV	PEM FC	ICEV	BEV	PEM FC	ICEV	BEV	PEM FC
Road: P, M & D	1.0	1.0	1.0	0.0073	0.0073	0.0073	0.216	0.22	0.22
Glider	3.2	3.2	3.2	0.0246	0.0246	0.0246	0.455	0.45	0.45
Drivetrain	1.3	1.6	1.6	0.0096	0.0088	0.0088	0.198	0.15	0.15
Car: M & D	0.8	0.8	0.8	0.0080	0.0078	0.0078	0.165	0.16	0.16
Li-ion bettery: P, M & D		3.8	0.3		0.0118	0.0008		0.22	0.01
PEM FC: P, M & D			2.3			0.0178			0.24
Operation Petrol	13.2			0.1526			2.265		
Operation UCTE		9.7	23.4		0.1014	0.2456		2.2	5.2
Operation Solar		1.9	4.6		0.015	0.037		0.93	2.3
Operation Wind		0.4	1.1		0.002	0.006		0.69	1.7
Operation Hydro		0.2	0.5		0.001	0.003		0.65	1.6

Table S25. Environmental performance in ReCiPe millipoints (m.points) and of micro combined heat and power (µ-CHP) plant powered with a PEM fuel cell or a stirling engine. System expansion is matched such that both µ-CHP plants provide equal amounts of heat and electricity.

	0.4 MJ Electricity and 0.5 MJ Heat	0.31 MJ Heat from natural gas	0.15 MJ Electricity and 0.81 MJ Heat	0.25 MJ Electricity, UCTE mix
ReCiPe (millipoints)	PEM FC	System expansion PEM FC	Stirling	System expansion Stirling
Climate change Human Health	1.901	0.630	1.872	1.144
Ozone depletion	0.001	0.000	0.001	0.000
Human toxicity	0.025	0.010	0.009	0.426
Photochemical oxidant formation	0.000	0.000	0.000	0.000
Particulate matter formation	0.085	0.030	0.130	0.288
Ionising radiation	0.000	0.000	0.000	0.011
Climate change Ecosystems	1.203	0.398	1.184	0.724
Terrestrial acidification	0.001	0.000	0.001	0.002
Freshwater eutrophication	0.000	0.000	0.000	0.004
Terrestrial ecotoxicity	0.000	0.000	0.000	0.001
Freshwater ecotoxicity	0.000	0.000	0.000	0.001
Marine ecotoxicity	0.000	0.000	0.000	0.000
Agricultural land occupation	0.001	0.001	0.000	0.016
Urban land occupation	0.001	0.001	0.001	0.006
Natural land transformation	0.033	0.011	0.033	0.014
Metal depletion	0.086	0.011	0.014	0.084
Fossil depletion	2.749	0.875	2.715	1.201
Total	6.086	1.967	5.961	3.923

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