Electronic Supplementary Material (ESI) for RSC Advances

Life Cycle Assessment to Measure the Environmental Performance of Catalysts and Directing Research in the Conversion of CO_2 into Commodity Chemicals: *a look at the potential for fuels from 'thin-air'*

O. Glyn Griffiths, Rhodri E. Owen, Justin P. O'Byrne, Davida Mattia, Matthew D. Jones and Marcelle C. McManus

Supporting Information

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Catalyst Preparation

A range of catalysts consisting of various metal loadings were prepared and analysed for this study. Metal loadings were calculated based on the metal content of the precursor compounds and measured relative to the initial weight of the silica catalyst support used. Table 3 details the metal loadings of the catalysts investigated with iron content increasing from 10 wt% to 40 wt% with up to 4wt% palladium added as a promoter. Other than the masses of the iron and palladium compounds used, the preparation of each catalyst proceeded *via* the same wet impregnation technique detailed in steps 1-7.

1 2.00 g of silica is dispersed in methanol and stirred using a magnetic stirrer.

2 A methanolic solution of iron nitrate is prepared using the appropriate mass (see table 1) of $Fe(NO_3)_3 \cdot 9H_2O$.

3 A solution of palladium acetate (not used for catalyst Fe20 synthesis) is also prepared by dissolving the required amount (see table 3) of $Pd(OAc)_2$ in methanol.

4 Each metal solution is added drop-wise to the dispersed silica support in turn.

5 The resulting mixture is then sonicated for 1 hour.

6 Methanol is removed using the combination of a heated water bath, rotary evaporator and vacuum pump until a dry powder is obtained. Water is used to condense the methanol, which is recovered for subsequent re-use.

Steps 1-6 are repeated for each catalyst until four batches of dry powder are formed.

7 Four batches of catalyst per operation of the high temperature furnace are heated to 450 °C and calcined at this temperature for 12 hours.

Catalyst Testing

Table 1 shows that the final catalyst masses, δ, is dependent on the desired amount of iron and palladium loadings respectively, and ranges from 2.35 to 3.98 g. The mass of silica support is kept constant at 2.00 g for each catalyst formation. For the catalytic process under investigation 1.00 g of catalyst is used during the reaction. It follows therefore that the synthesis of higher masses for the same procedure (same use of solvent, equipment and electricity), will result in proportionally reduced embodied environmental impacts inherited by the finished catalyst powder. LCA results take account of varying catalyst masses.

Catalyst testing occurs in a horizontal furnace, with an approximate heating region of 700 mm and maximum internal passageway diameter of 75 mm. 1.0 g of catalyst is placed within a stainless steel tube with a diameter of 6.35 mm. The sample is kept packed and in place through the use of quartz wool which allows the unhindered passage of reactant gases and formed products.

Once the furnace is heated to 300 °C pre-treatment commences, this involves the reduction of the calcined catalyst powder under a pure flow of 50 standard cubic centimetres per minute (sccm) of hydrogen for 2 hours. After pre-treatment the furnace is further heated to 370 °C and the flow of hydrogen is reduced to 6 sccm and CO_2 is introduced at a flow of 2 sccm. The reaction stages are modelled as the following steps (8-11), and follow on from the catalyst preparation steps

8 The prepared catalyst is placed inside the horizontal furnace and is heated to 300 °C.

9 Catalyst pre-treated under a flow of 50 sccm H_2 at 300 °C for 2 hours.

10 Horizontal furnace temperature increased to 370 °C.

11 Once reaction temperature is reached the flow of H_2 is reduced and CO_2 is introduced, catalysis commences.

All catalyst formation and reaction steps, 1 to 11, are modelled discreetly in the LCA of the entire catalysis process under investigation.

Catalyst Composition and Masses

Table 1 The formed catalyst compositions and masses.

Name	Composition	$Fe(NO)_3.9H_2O$/g	$Pd(OAc)_2$/g	Final Catalyst mass,δ/g
Fe20	**20**wt%Fe/SiO_2	3.618	0.000	2.72
Fe10Pd1	**10**wt%Fe/01wt%Pd/SiO_2	1.626	0.047	2.35
Fe20Pd1*	**20**wt%Fe/01wt%Pd/SiO_2	3.664	0.053	2.75
Fe30Pd1	**30**wt%Fe/01wt%Pd/SiO_2	6.292	0.061	3.28
Fe40Pd1	**40**wt%Fe/01wt%Pd/SiO_2	9.811	0.071	3.98
Pd1Fe20*	20wt%Fe/**01**wt%Pd/SiO_2	3.664	0.053	2.75
Pd2Fe20	20wt%Fe/**02**wt%Pd/SiO_2	3.711	0.108	2.79
Pd3Fe20	20wt%Fe/**03**wt%Pd/SiO_2	3.759	0.164	2.83
Pd4Fe20	20wt%Fe/**04**wt%Pd/SiO_2	3.808	0.222	2.87

**these catalysts are the same, modelled separately to show iron and palladium trends*

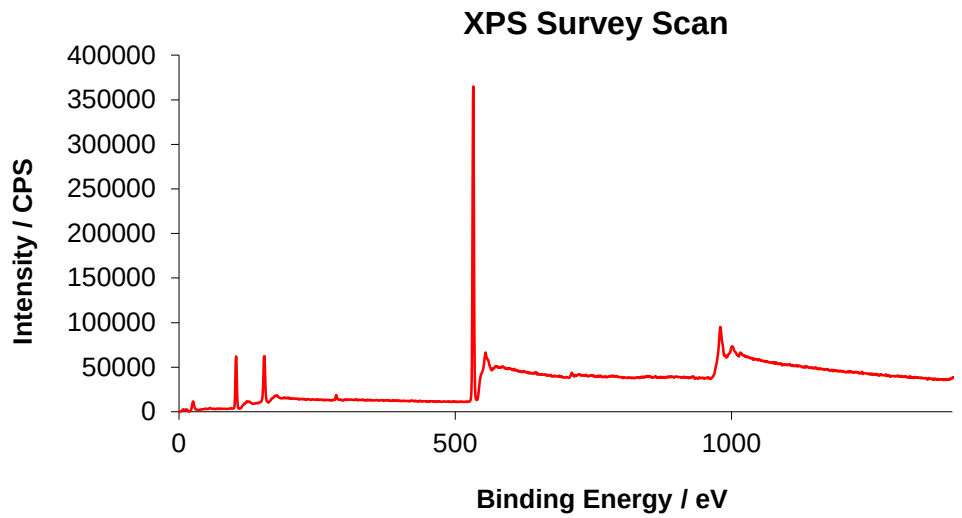
X-ray photoelectron spectroscopy Examples

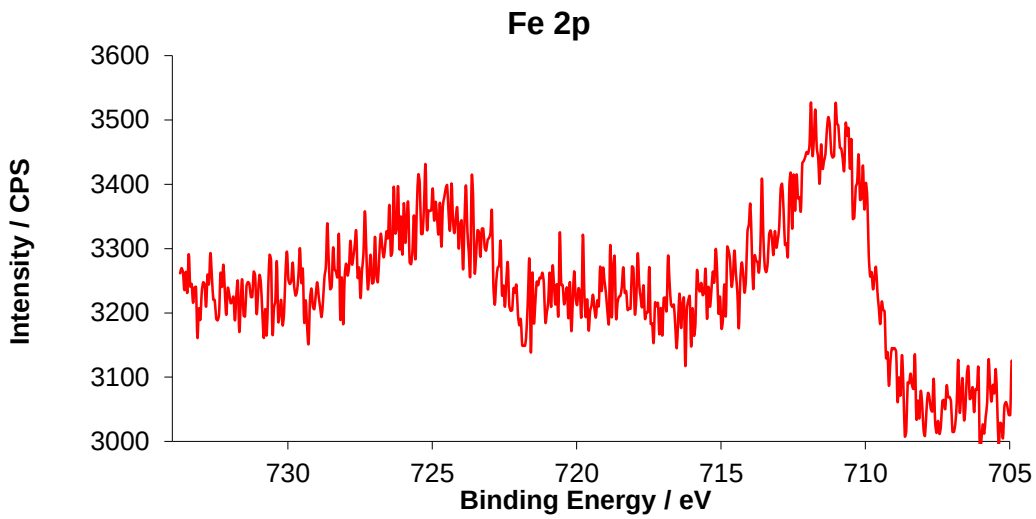
XPS - 20wt%Fe/SiO_2

XPS studies conducted on the 20wt%Fe/SiO_2 catalyst before use revealed that iron is present mainly in the Fe_2O_3 form.

Table of XPS Results

Catalyst	Binding Energy (eV)	Composition (atom %)			
	Fe 2p	Fe 2p	Si 2p	O 1s	C 1s
20wt%Fe/SiO_2	711.0	0.382	31.228	65.767	2.623



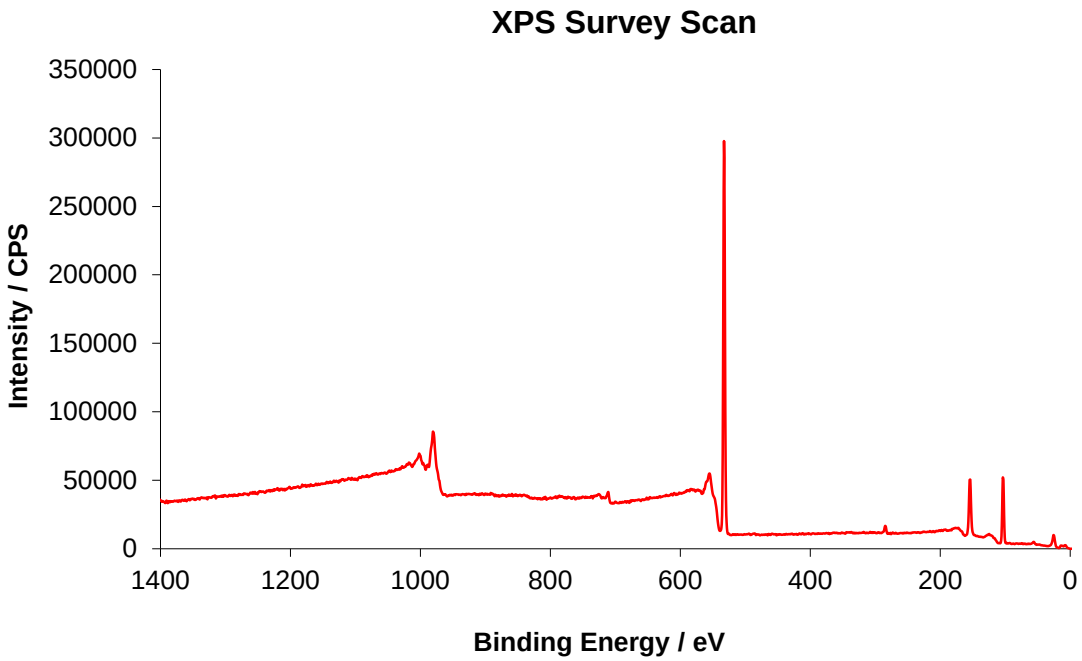


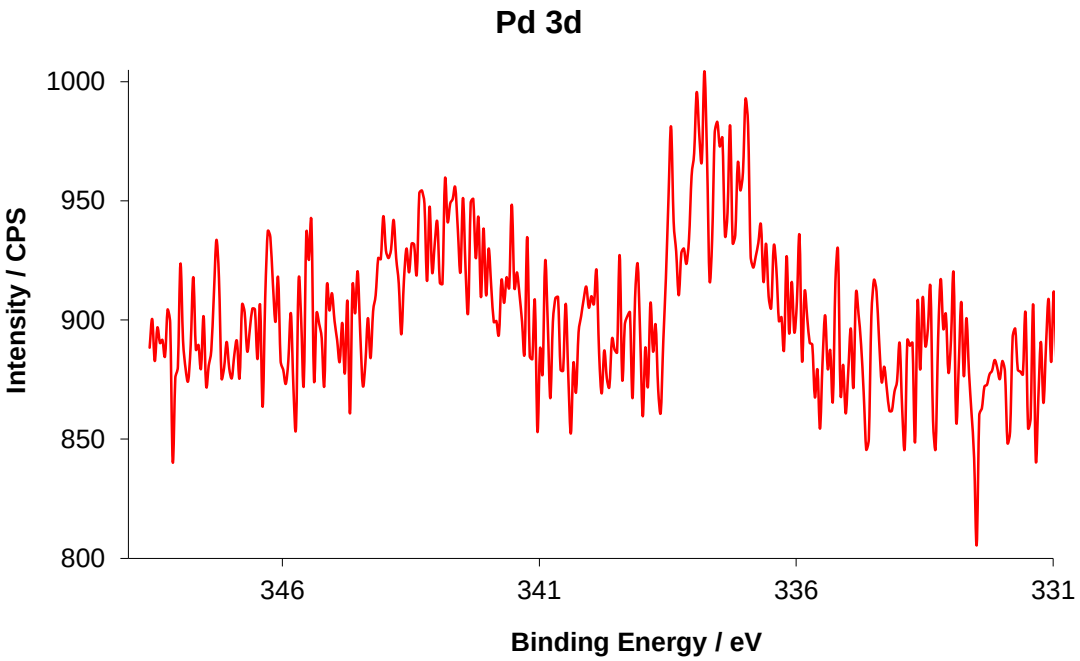
XPS - 20wt%Fe/1wt%Pd/SiO_2

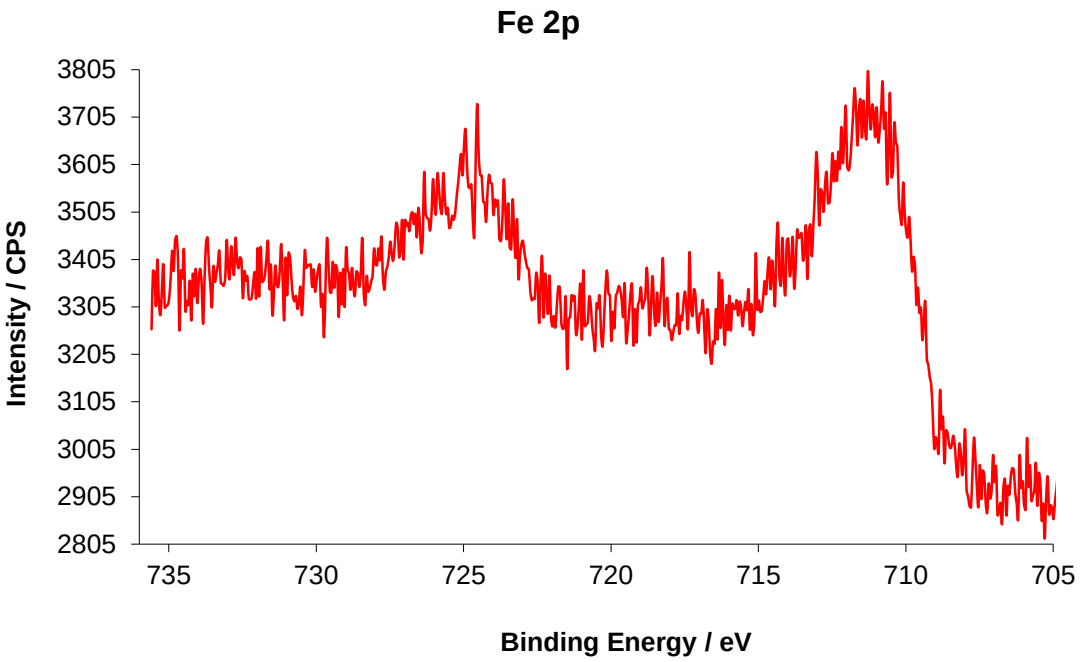
XPS studies conducted on the 20wt%Fe/1wt%Pd/SiO_2 catalyst before use revealed that iron is present mainly in the Fe_2O_3 form and palladium mainly as the oxide PdO.

Table of XPS Results

Catalyst	Binding Energy (eV)		Composition (atom %)				
	Fe 2p	Pd 3d	Pd 3d	Fe 2p	Si 2p	O 1s	C 1s
20wt%Fe/1wt%Pd/SiO_2	710.8	337.8	0.1	0.297	30.463	65.209	3.931

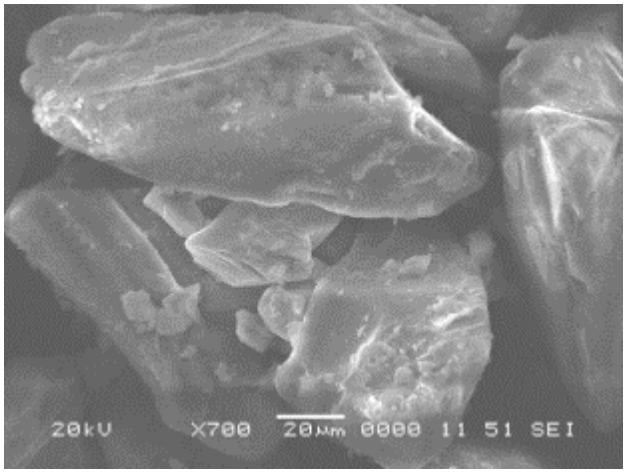




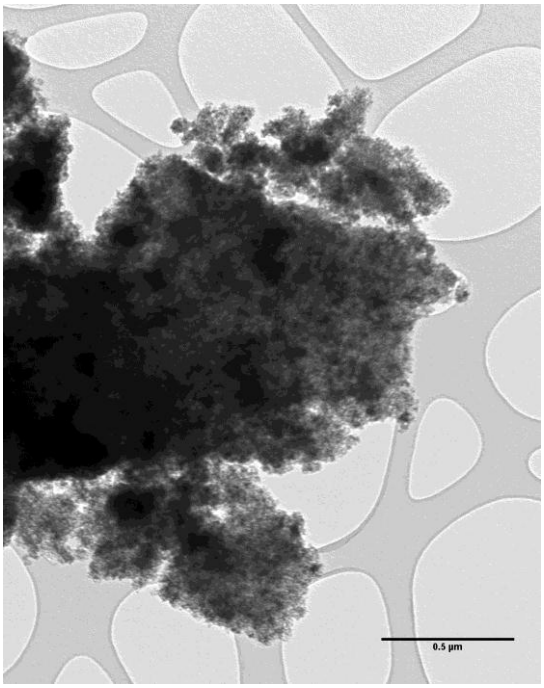


Example Catalyst Characterisation Electron Microscopy Images

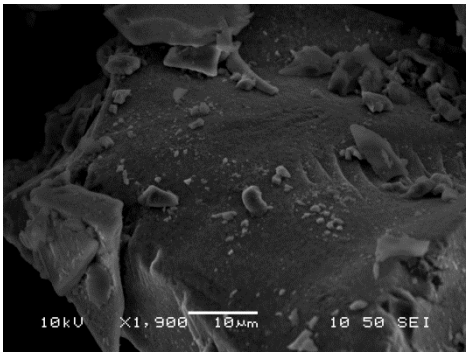
- SEM recorded on a JEOL 6480LV at 5-20 kV.
- TEM recorded using a JEOL 1200 operated at 120 kV.
- Samples were prepared in ethanol and deposited onto copper or nickel grids.

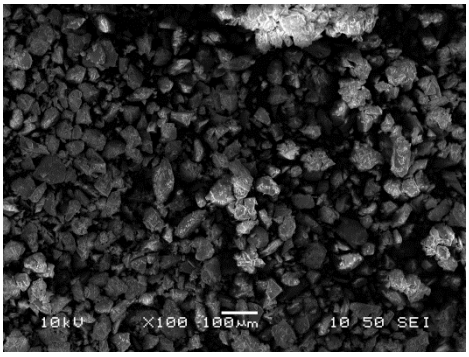


SEM Image Recorded for 20wt%Fe/SiO_2

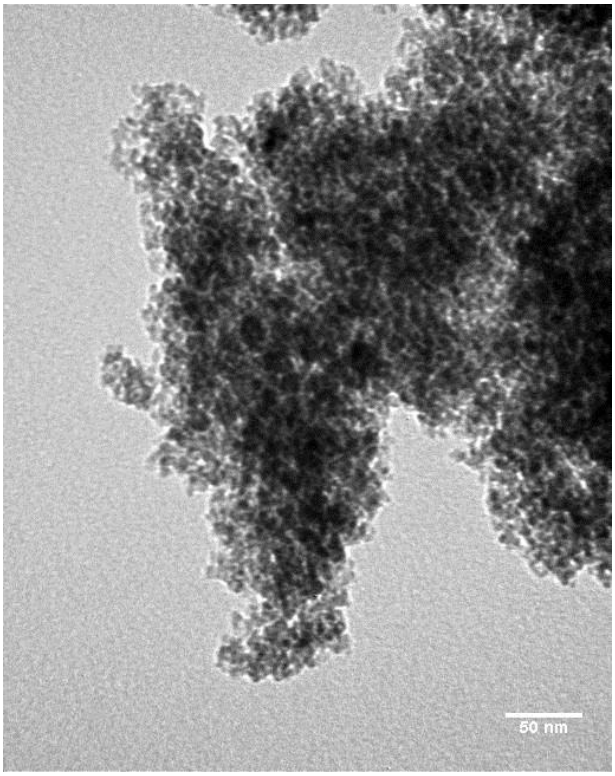


TEM Image Recorded for 20wt%Fe/SiO_2





SEM Images Recorded for 20wt%Fe/1wt%Pd/SiO_2



TEM Image Recorded for 20wt%Fe/1wt%Pd/SiO_2

Relative surface areas of catalysts

BET Measurements Recorded for Catalysts

Catalyst	10wt%Fe/1wt%Pd /SiO_2	20wt%Fe/1wt%Pd /SiO_2	30wt%Fe/1wt%Pd /SiO_2	40wt%Fe/1wt%Pd /SiO_2
Surface Area (m^2g^{-1})	378.8	281.1	269.5	249.1

Catalyst	20wt%Fe/1wt%Pd /SiO_2	20wt%Fe/2wt%Pd /SiO_2	20wt%Fe/3wt%Pd /SiO_2	20wt%Fe/4wt%Pd /SiO_2
Surface Area (m^2g^{-1})	281.1	311.3	325.2	330.7

Characterised data for the synthesis of the different catalysts

Title:	Comparing product stages
Method:	ReCiPe Midpoint (H) V1.05 / Europe ReCiPe H
Indicator:	Characterisation
Skip categories:	Never
Relative mode:	None
Exclude infrastructure processes:	No
Exclude long-term emissions:	No

C = Chemicals, E= Electricity usage, I = Infrastructure Contributions, M = iron and/or palladium addition

Impact category	Unit	Cat_Fe_Synthesis_C	Cat_Fe_Synthesis_E	Cat_Fe_Synthesis_I	Cat_Fe_Synthesis_M
Climate change	kg CO2 eq	1.299E-02	5.936E-01	4.001E-02	8.817E-03
Ozone depletion	kg CFC-11 eq	2.518E-09	1.494E-08	9.505E-07	2.887E-10
Human toxicity	kg 1,4-DB eq	1.964E-03	1.237E-01	1.743E-02	6.836E-04
Photochemical oxidant formation	kg NMVOC	2.929E-05	1.199E-03	3.504E-05	1.681E-05
Particulate matter formation	kg PM10 eq	1.165E-05	5.976E-04	3.745E-05	7.269E-06
Ionising radiation	kg U235 eq	1.193E-03	2.721E-01	2.644E-03	1.464E-04
Terrestrial acidification	kg SO2 eq	4.087E-05	1.852E-03	1.170E-04	3.002E-05
Freshwater eutrophication	kg P eq	2.073E-06	1.685E-04	1.087E-05	3.926E-07
Marine eutrophication	kg N eq	7.268E-06	4.360E-04	8.647E-06	7.204E-06
Terrestrial ecotoxicity	kg 1,4-DB eq	1.260E-06	4.102E-05	1.912E-06	3.605E-07
Freshwater ecotoxicity	kg 1,4-DB eq	5.421E-05	2.564E-03	3.165E-04	9.574E-06
Marine ecotoxicity	kg 1,4-DB eq	4.096E-05	2.747E-03	3.300E-04	1.300E-05
Agricultural land occupation	m2a	9.806E-05	1.091E-02	2.531E-04	4.458E-05
Urban land occupation	m2a	5.226E-05	2.572E-03	1.139E-04	9.925E-06
Natural land transformation	m2	6.136E-06	1.175E-04	1.606E-06	7.657E-07
Water depletion	m3	1.692E-03	3.306E-03	1.206E-04	1.097E-05
Metal depletion	kg Fe eq	4.143E-04	2.870E-03	8.562E-03	2.113E-04
Fossil depletion	kg oil eq	1.359E-02	1.847E-01	2.759E-03	8.405E-04

Impact category	Unit	Cat_Fe10_Synthesis_C	Cat_Fe10_Synthesis_E	Cat_Fe10_Synthesis_I	Cat_Fe10_Synthesis_M
Climate change	kg CO2 eq	1.504E-02	6.872E-01	4.631E-02	9.772E-02
Ozone depletion	kg CFC-11 eq	2.915E-09	1.729E-08	1.100E-06	8.630E-09
Human toxicity	kg 1,4-DB eq	2.273E-03	1.431E-01	2.018E-02	3.170E-01
Photochemical oxidant formation	kg NMVOC	3.391E-05	1.387E-03	4.056E-05	4.792E-03
Particulate matter formation	kg PM10 eq	1.349E-05	6.918E-04	4.335E-05	1.146E-02
Ionising radiation	kg U235 eq	1.381E-03	3.150E-01	3.061E-03	4.306E-02
Terrestrial acidification	kg SO2 eq	4.731E-05	2.144E-03	1.354E-04	5.639E-02
Freshwater eutrophication	kg P eq	2.400E-06	1.950E-04	1.259E-05	2.046E-04
Marine eutrophication	kg N eq	8.413E-06	5.047E-04	1.001E-05	1.046E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.458E-06	4.748E-05	2.214E-06	1.484E-05
Freshwater ecotoxicity	kg 1,4-DB eq	6.275E-05	2.968E-03	3.664E-04	1.050E-02
Marine ecotoxicity	kg 1,4-DB eq	4.741E-05	3.180E-03	3.821E-04	1.035E-02
Agricultural land occupation	m2a	1.135E-04	1.263E-02	2.930E-04	2.013E-03
Urban land occupation	m2a	6.049E-05	2.978E-03	1.319E-04	1.618E-03
Natural land transformation	m2	7.103E-06	1.360E-04	1.859E-06	1.505E-05
Water depletion	m3	1.959E-03	3.827E-03	1.396E-04	2.950E-03
Metal depletion	kg Fe eq	4.796E-04	3.322E-03	9.912E-03	4.303E-02
Fossil depletion	kg oil eq	1.573E-02	2.138E-01	3.194E-03	2.948E-02

Impact category	Unit	Cat_Fe20_Synthesis_C	Cat_Fe20_Synthesis_E	Cat_Fe20_Synthesis_I	Cat_Fe20_Synthesis_M
Climate change	kg CO2 eq	1.285E-02	5.872E-01	3.957E-02	9.847E-02
Ozone depletion	kg CFC-11 eq	2.490E-09	1.478E-08	9.402E-07	8.452E-09
Human toxicity	kg 1,4-DB eq	1.943E-03	1.223E-01	1.724E-02	3.055E-01
Photochemical oxidant formation	kg NMVOC	2.897E-05	1.185E-03	3.466E-05	4.622E-03
Particulate matter formation	kg PM10 eq	1.152E-05	5.911E-04	3.704E-05	1.103E-02
Ionising radiation	kg U235 eq	1.180E-03	2.691E-01	2.615E-03	4.153E-02
Terrestrial acidification	kg SO2 eq	4.042E-05	1.832E-03	1.157E-04	5.430E-02
Freshwater eutrophication	kg P eq	2.050E-06	1.666E-04	1.076E-05	1.972E-04
Marine eutrophication	kg N eq	7.189E-06	4.313E-04	8.553E-06	1.043E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.246E-06	4.057E-05	1.891E-06	1.447E-05
Freshwater ecotoxicity	kg 1,4-DB eq	5.362E-05	2.536E-03	3.131E-04	1.012E-02
Marine ecotoxicity	kg 1,4-DB eq	4.051E-05	2.717E-03	3.265E-04	9.969E-03
Agricultural land occupation	m2a	9.699E-05	1.079E-02	2.504E-04	1.960E-03
Urban land occupation	m2a	5.169E-05	2.544E-03	1.127E-04	1.563E-03
Natural land transformation	m2	6.069E-06	1.162E-04	1.588E-06	1.488E-05
Water depletion	m3	1.674E-03	3.270E-03	1.193E-04	2.845E-03
Metal depletion	kg Fe eq	4.098E-04	2.839E-03	8.469E-03	4.153E-02
Fossil depletion	kg oil eq	1.344E-02	1.827E-01	2.729E-03	2.880E-02

Impact category	Unit	Cat_Fe30_Synthesis_C	Cat_Fe30_Synthesis_E	Cat_Fe30_Synthesis_I	Cat_Fe30_Synthesis_M
Climate change	kg CO2 eq	1.077E-02	4.920E-01	3.316E-02	9.885E-02
Ozone depletion	kg CFC-11 eq	2.087E-09	1.238E-08	7.878E-07	8.260E-09
Human toxicity	kg 1,4-DB eq	1.628E-03	1.025E-01	1.445E-02	2.939E-01
Photochemical oxidant formation	kg NMVOC	2.428E-05	9.933E-04	2.904E-05	4.449E-03
Particulate matter formation	kg PM10 eq	9.657E-06	4.953E-04	3.104E-05	1.061E-02
Ionising radiation	kg U235 eq	9.888E-04	2.255E-01	2.191E-03	3.998E-02
Terrestrial acidification	kg SO2 eq	3.387E-05	1.535E-03	9.698E-05	5.219E-02
Freshwater eutrophication	kg P eq	1.718E-06	1.396E-04	9.012E-06	1.897E-04
Marine eutrophication	kg N eq	6.023E-06	3.614E-04	7.167E-06	1.037E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.044E-06	3.400E-05	1.585E-06	1.408E-05
Freshwater ecotoxicity	kg 1,4-DB eq	4.493E-05	2.125E-03	2.623E-04	9.726E-03
Marine ecotoxicity	kg 1,4-DB eq	3.394E-05	2.277E-03	2.735E-04	9.585E-03
Agricultural land occupation	m2a	8.127E-05	9.040E-03	2.098E-04	1.905E-03
Urban land occupation	m2a	4.331E-05	2.132E-03	9.444E-05	1.507E-03
Natural land transformation	m2	5.086E-06	9.736E-05	1.331E-06	1.466E-05
Water depletion	m3	1.402E-03	2.740E-03	9.998E-05	2.739E-03
Metal depletion	kg Fe eq	3.434E-04	2.378E-03	7.097E-03	4.001E-02
Fossil depletion	kg oil eq	1.126E-02	1.531E-01	2.287E-03	2.807E-02

Impact category	Unit	Cat_Fe40_Synthesis_C	Cat_Fe40_Synthesis_E	Cat_Fe40_Synthesis_I	Cat_Fe40_Synthesis_M
Climate change	kg CO2 eq	8.860E-03	4.049E-01	2.729E-02	9.927E-02
Ozone depletion	kg CFC-11 eq	1.717E-09	1.019E-08	6.483E-07	8.087E-09
Human toxicity	kg 1,4-DB eq	1.339E-03	8.434E-02	1.189E-02	2.833E-01
Photochemical oxidant formation	kg NMVOC	1.998E-05	8.175E-04	2.390E-05	4.291E-03
Particulate matter formation	kg PM10 eq	7.947E-06	4.076E-04	2.554E-05	1.021E-02
Ionising radiation	kg U235 eq	8.137E-04	1.856E-01	1.803E-03	3.856E-02
Terrestrial acidification	kg SO2 eq	2.787E-05	1.263E-03	7.981E-05	5.027E-02
Freshwater eutrophication	kg P eq	1.414E-06	1.149E-04	7.417E-06	1.828E-04
Marine eutrophication	kg N eq	4.957E-06	2.974E-04	5.898E-06	1.032E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	8.592E-07	2.798E-05	1.304E-06	1.372E-05
Freshwater ecotoxicity	kg 1,4-DB eq	3.697E-05	1.749E-03	2.159E-04	9.369E-03
Marine ecotoxicity	kg 1,4-DB eq	2.793E-05	1.874E-03	2.251E-04	9.235E-03
Agricultural land occupation	m2a	6.688E-05	7.440E-03	1.727E-04	1.855E-03
Urban land occupation	m2a	3.564E-05	1.755E-03	7.772E-05	1.455E-03
Natural land transformation	m2	4.185E-06	8.012E-05	1.095E-06	1.447E-05
Water depletion	m3	1.154E-03	2.255E-03	8.228E-05	2.642E-03
Metal depletion	kg Fe eq	2.826E-04	1.957E-03	5.840E-03	3.862E-02
Fossil depletion	kg oil eq	9.268E-03	1.260E-01	1.882E-03	2.742E-02

Impact category	Unit	Cat_Pd1_Synthesis_C	Cat_Pd1_Synthesis_E	Cat_Pd1_Synthesis_I	Cat_Pd1_Synthesis_M
Climate change	kg CO2 eq	1.285E-02	5.872E-01	3.957E-02	9.847E-02
Ozone depletion	kg CFC-11 eq	2.490E-09	1.478E-08	9.402E-07	8.452E-09
Human toxicity	kg 1,4-DB eq	1.943E-03	1.223E-01	1.724E-02	3.055E-01
Photochemical oxidant formation	kg NMVOC	2.897E-05	1.185E-03	3.466E-05	4.622E-03
Particulate matter formation	kg PM10 eq	1.152E-05	5.911E-04	3.704E-05	1.103E-02
Ionising radiation	kg U235 eq	1.180E-03	2.691E-01	2.615E-03	4.153E-02
Terrestrial acidification	kg SO2 eq	4.042E-05	1.832E-03	1.157E-04	5.430E-02
Freshwater eutrophication	kg P eq	2.050E-06	1.666E-04	1.076E-05	1.972E-04
Marine eutrophication	kg N eq	7.189E-06	4.313E-04	8.553E-06	1.043E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.246E-06	4.057E-05	1.891E-06	1.447E-05
Freshwater ecotoxicity	kg 1,4-DB eq	5.362E-05	2.536E-03	3.131E-04	1.012E-02
Marine ecotoxicity	kg 1,4-DB eq	4.051E-05	2.717E-03	3.265E-04	9.969E-03
Agricultural land occupation	m2a	9.699E-05	1.079E-02	2.504E-04	1.960E-03
Urban land occupation	m2a	5.169E-05	2.544E-03	1.127E-04	1.563E-03
Natural land transformation	m2	6.069E-06	1.162E-04	1.588E-06	1.488E-05
Water depletion	m3	1.674E-03	3.270E-03	1.193E-04	2.845E-03
Metal depletion	kg Fe eq	4.098E-04	2.839E-03	8.469E-03	4.153E-02
Fossil depletion	kg oil eq	1.344E-02	1.827E-01	2.729E-03	2.880E-02

Impact category	Unit	Cat_Pd2_Synthesis_C	Cat_Pd2_Synthesis_E	Cat_Pd2_Synthesis_I	Cat_Pd2_Synthesis_M
Climate change	kg CO2 eq	1.264E-02	5.775E-01	3.892E-02	1.879E-01
Ozone depletion	kg CFC-11 eq	2.449E-09	1.453E-08	9.247E-07	1.659E-08
Human toxicity	kg 1,4-DB eq	1.911E-03	1.203E-01	1.696E-02	6.094E-01
Photochemical oxidant formation	kg NMVOC	2.850E-05	1.166E-03	3.409E-05	9.213E-03
Particulate matter formation	kg PM10 eq	1.133E-05	5.814E-04	3.643E-05	2.203E-02
Ionising radiation	kg U235 eq	1.161E-03	2.647E-01	2.572E-03	8.280E-02
Terrestrial acidification	kg SO2 eq	3.976E-05	1.802E-03	1.138E-04	1.084E-01
Freshwater eutrophication	kg P eq	2.016E-06	1.639E-04	1.058E-05	3.934E-04
Marine eutrophication	kg N eq	7.070E-06	4.242E-04	8.412E-06	2.011E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.225E-06	3.990E-05	1.860E-06	2.854E-05
Freshwater ecotoxicity	kg 1,4-DB eq	5.273E-05	2.494E-03	3.079E-04	2.020E-02
Marine ecotoxicity	kg 1,4-DB eq	3.984E-05	2.672E-03	3.211E-04	1.990E-02
Agricultural land occupation	m2a	9.539E-05	1.061E-02	2.463E-04	3.871E-03
Urban land occupation	m2a	5.084E-05	2.503E-03	1.109E-04	3.112E-03
Natural land transformation	m2	5.969E-06	1.143E-04	1.562E-06	2.894E-05
Water depletion	m3	1.646E-03	3.216E-03	1.174E-04	5.671E-03
Metal depletion	kg Fe eq	4.030E-04	2.792E-03	8.330E-03	8.274E-02
Fossil depletion	kg oil eq	1.322E-02	1.797E-01	2.684E-03	5.667E-02

Impact category	Unit	Cat_Pd3_Synthesis_C	Cat_Pd3_Synthesis_E	Cat_Pd3_Synthesis_I	Cat_Pd3_Synthesis_M
Climate change	kg CO2 eq	1.246E-02	5.694E-01	3.838E-02	2.770E-01
Ozone depletion	kg CFC-11 eq	2.415E-09	1.433E-08	9.118E-07	2.471E-08
Human toxicity	kg 1,4-DB eq	1.884E-03	1.186E-01	1.672E-02	9.125E-01
Photochemical oxidant formation	kg NMVOC	2.810E-05	1.150E-03	3.361E-05	1.379E-02
Particulate matter formation	kg PM10 eq	1.118E-05	5.733E-04	3.592E-05	3.299E-02
Ionising radiation	kg U235 eq	1.144E-03	2.610E-01	2.536E-03	1.240E-01
Terrestrial acidification	kg SO2 eq	3.920E-05	1.777E-03	1.122E-04	1.624E-01
Freshwater eutrophication	kg P eq	1.988E-06	1.616E-04	1.043E-05	5.891E-04
Marine eutrophication	kg N eq	6.971E-06	4.182E-04	8.295E-06	2.977E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.208E-06	3.935E-05	1.834E-06	4.256E-05
Freshwater ecotoxicity	kg 1,4-DB eq	5.200E-05	2.460E-03	3.036E-04	3.025E-02
Marine ecotoxicity	kg 1,4-DB eq	3.929E-05	2.635E-03	3.166E-04	2.980E-02
Agricultural land occupation	m2a	9.406E-05	1.046E-02	2.428E-04	5.776E-03
Urban land occupation	m2a	5.013E-05	2.468E-03	1.093E-04	4.656E-03
Natural land transformation	m2	5.886E-06	1.127E-04	1.540E-06	4.297E-05
Water depletion	m3	1.623E-03	3.171E-03	1.157E-04	8.490E-03
Metal depletion	kg Fe eq	3.974E-04	2.753E-03	8.213E-03	1.238E-01
Fossil depletion	kg oil eq	1.303E-02	1.772E-01	2.646E-03	8.447E-02

Impact category	Unit	Cat_Pd4_Synthesis_C	Cat_Pd4_Synthesis_E	Cat_Pd4_Synthesis_I	Cat_Pd4_Synthesis_M
Climate change	kg CO2 eq	1.228E-02	5.614E-01	3.783E-02	3.661E-01
Ozone depletion	kg CFC-11 eq	2.381E-09	1.413E-08	8.989E-07	3.282E-08
Human toxicity	kg 1,4-DB eq	1.857E-03	1.169E-01	1.649E-02	1.215E+00
Photochemical oxidant formation	kg NMVOC	2.770E-05	1.133E-03	3.314E-05	1.837E-02
Particulate matter formation	kg PM10 eq	1.102E-05	5.651E-04	3.541E-05	4.395E-02
Ionising radiation	kg U235 eq	1.128E-03	2.573E-01	2.500E-03	1.651E-01
Terrestrial acidification	kg SO2 eq	3.865E-05	1.752E-03	1.106E-04	2.163E-01
Freshwater eutrophication	kg P eq	1.960E-06	1.593E-04	1.028E-05	7.847E-04
Marine eutrophication	kg N eq	6.873E-06	4.123E-04	8.177E-06	3.941E-04
Terrestrial ecotoxicity	kg 1,4-DB eq	1.191E-06	3.879E-05	1.808E-06	5.658E-05
Freshwater ecotoxicity	kg 1,4-DB eq	5.126E-05	2.425E-03	2.993E-04	4.029E-02
Marine ecotoxicity	kg 1,4-DB eq	3.873E-05	2.598E-03	3.121E-04	3.969E-02
Agricultural land occupation	m2a	9.273E-05	1.032E-02	2.394E-04	7.680E-03
Urban land occupation	m2a	4.942E-05	2.433E-03	1.078E-04	6.199E-03
Natural land transformation	m2	5.803E-06	1.111E-04	1.518E-06	5.699E-05
Water depletion	m3	1.600E-03	3.126E-03	1.141E-04	1.131E-02
Metal depletion	kg Fe eq	3.918E-04	2.714E-03	8.097E-03	1.649E-01
Fossil depletion	kg oil eq	1.285E-02	1.746E-01	2.609E-03	1.122E-01

Characterised In-Use, Impacts per hour

Title:	Comparing product stages
Method:	ReCiPe Midpoint (H) V1.05 / Europe ReCiPe H
Indicator:	Characterisation
Skip categories:	Never
Relative mode:	None
Exclude infrastructure processes:	No
Exclude long-term emissions:	No

Impact category	Unit	Per hour of reaction
Climate change	kg CO2 eq	0.065092023
Ozone depletion	kg CFC-11 eq	1.66E-09
Human toxicity	kg 1,4-DB eq	0.014246928
Photochemical oxidant formation	kg NMVOC	0.0001329
Particulate matter formation	kg PM10 eq	6.82E-05
Ionising radiation	kg U235 eq	0.029735521
Terrestrial acidification	kg SO2 eq	0.000212087
Freshwater eutrophication	kg P eq	1.89E-05
Marine eutrophication	kg N eq	4.80E-05
Terrestrial ecotoxicity	kg 1,4-DB eq	4.61E-06
Freshwater ecotoxicity	kg 1,4-DB eq	0.000296336
Marine ecotoxicity	kg 1,4-DB eq	0.000317586
Agricultural land occupation	m2a	0.00120403
Urban land occupation	m2a	0.000285997
Natural land transformation	m2	1.29E-05
Water depletion	m3	0.000365253
Metal depletion	kg Fe eq	0.000810515
Fossil depletion	kg oil eq	0.020294775

Hydrocarbon (HC) Offsets

The hydrocarbons assessed in this study are all present in the Ecoinvent V2.2 database .[1]

HCs	**Methane**	**Ethene**	**Ethane**	**Propene**	**Propane**	**Iso-Butane / n-Butane**	**Pentane**	**Hexane**	**C7>**
Modelled Dataset. Ecoinvent V2.2	*Methane, 96 vol-%, from biogas, production mix, at service station/CH U*	*Ethene (ethylene), from steam cracking, production mix, at plant, gaseous EU-27 S*		*Propane/ butane, at refinery/RER S*		**Average of:** *Propane/ butane, at refinery/RER S* **and:** *Butanes from butenes, at plant/RER U*	*Pentane, at plant/RER U*	*Hexane, at plant/RER U*	*Heptane, at plant/RER U*

Method: ReCiPe Midpoint (H) V1.05 / Europe ReCiPe H / Normalisation

HCs	**Methane**	**Ethene**	**Ethane**	**Propene**	**Propane**	**Iso-Butane**	**N-Butane**	**Pentane**	**Hexane**	**C7>**
Total impacts / gram	4.79E-06	1.47E-06	1.47E-06	1.42E-05	1.42E-05	1.2E-05	1.2E-05	1.76E-06	1.62E-05	1.62E-05

The above values are used in the paper when ‘HC offset’ is discussed.

Chemical Dataset Modelling

Taken from paper: The allocation of total impacts to the desired products is deemed a justifiable assumption, since the production of NO is of lesser economic value than the metal compounds formed. However, if allocation on a mass basis were to occur then $Fe(NO_3).9H_2O$ and $Pd(OAc)_2$ would have 89% and 71.5% of the impacts reported in this study respectively.

Palladium Acetate Created Dataset

Name: Palladium Acetate 0.0001g 3

Image

Comment

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Palladium, at regional storage/RER U	4.74016E-5	g	Undefined				...closest dataset available. Seems to capture most aspects documented in Ullmann's encyclopedia.
Nitric acid, 50% in H2O, at plant/RER U	0.000224536	g	Undefined				...double calculated amount due to 50% dilution
Acetic acid, 98% in H2O, at plant/RER U	5.34964E-5	g	Undefined				-this acetic acid is a dataset that matches the most common industrial process route.
Chemical plant, organics/RER/I U	0.0000000004*0.0001*0.001 = 4E-17	p					
(Insert line here)							

Processes	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Heat, unspecific, in chemical plant/RER U	0.03825725	kJ	Undefined				Using specific heat capacities and 5 degree drop per minute assumption

Iron Nitrate Created Dataset

Name: Iron Nitrate 0.0001g 2

Image:

Comment: with plant

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Iron scrap, at plant/RER U	2.30899E-5	g	Undefined				
Nitric acid, 50% in H2O, at plant/RER U	0.000208428	g	Undefined				...double calculated quantity due to 50% dilution
Chemical plant, organics/RER/I U	0.0000000004*0.0001*0.001 = 4E-17	p					

Chromatography Grade Silica Created Dataset

Name: 2013 Silica [2 grams]

Image:

Comment: Chromatography grade, formed via precipitation reaction.

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Sodium silicate, furnace process, pieces, at plant/RER U	4.063064622	g	Undefined				Verified by pubchem 'open hearth formation'
Sulphuric acid, liquid, at plant/RER U	3.264710973	g	Undefined				Verified from pubchem ' sulphuric gas'
Silicone plant/RER/I U	0.0000000004*0.002 = 8E-13	p					

Infrastructure Datasets Created

Infrastructure contributions per batch of catalyst formed

Modelled infrastructure operation

Modelled piece of equipment	Lifetime [yrs.]	Operations/ day	Impacts per use*	Resultant embodied impact per use*
Mechanical Stirrer	10	2	$\frac{1}{\partial}$	$4.89 \times 10^{-5}. \frac{1}{\partial}$
Sonicator Bath	10	2	$\frac{1}{\partial}$	$4.89 \times 10^{-5}. \frac{1}{\partial}$
Rotary evaporator and water bath	15	2	$\frac{1}{\partial}$	$3.26 \times 10^{-5}. \frac{1}{\partial}$
Vacuum pump	10	2	$\frac{1}{\partial}$	$4.89 \times 10^{-5}. \frac{1}{\partial}$
High temperature furnace	15	2	$\frac{1}{4\partial}$	$8.15 \times 10^{-6}. \frac{1}{4\partial}$
Horizontal furnace	25	2	1	5.48×10^{-5}

**Where ∂ is equal to the final mass of the formed catalyst (see Table 2).*

Similarly the equipment in-use, per hour, impact is modelled in the LCA.

Temperature Controller

Name: Furnace Large Controller

Image:

Comment: 17-09-2012, updated from photogrpahs of controller
**used for the first time with FT LCA
07/01/2013

Status: Draft

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Capacitor, electrolyte type, < 2cm height, at plant/GLO U	2.99	g	Undefined				
Capacitor, SMD type, surface-mounting, at plant/GLO U	1.665	g	Undefined				
Connector, clamp connection, at plant/GLO U	3	g	Undefined				
Diode, glass-, SMD type, surface mounting, at plant/GLO U	0.5	g	Undefined				
Inductor, ring core choke type, at plant/GLO U	3	g	Undefined				
Inductor, ring core choke type, at plant/GLO U	3	g	Undefined				used to model relay
Integrated circuit, IC, logic type, at plant/GLO U	1.7	g	Undefined				
Light emitting diode, LED, at plant/GLO U	6.8	g	Undefined				
Resistor, metal film type, through-hole mounting, at plant/GLO U	0.2	g	Undefined				
Resistor, metal film type, through-hole mounting, at plant/GLO U	1	g	Undefined				used to model thermistor
Resistor, SMD type, surface mounting, at plant/GLO U	0.765	g	Undefined				
Transformer, low voltage use, at plant/GLO U	33.6	g	Undefined				
Printed wiring board, surface mount, lead-containing surface, at plant/GLO U	0.036/2 = 0.018	m2					
Printed wiring board, through-hole, lead-containing surface, at plant/GLO U	0.036/2 = 0.018	m2					
High density polyethylene resin, at plant/RNA	150	g	Undefined				
Steel, converter, low-alloyed, at plant/RER U	150	g	Undefined				
Synthetic rubber, at plant/RER U	3	g	Undefined				buttons and gaskets
Cable, ribbon cable, 20-pin, with plugs, at plant/GLO U	200	g	Undefined				
Solder, bar, Sn95.5Ag3.9Cu0.6, for electronics industry, at plant/GLO U	3	g	Undefined				

High Temperature Furnace

Name: Furnace 1100C

Image:

Comment: Data based, on technical data sheet and discussion with managing director of *** furnaces 20/1/12. Total mass 22kg
**new/amended datasets

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Steel, converter, unalloyed, at plant/RER U	0	kg	Undefined				
Galvanized steel sheet, at plant/RNA	11	kg	Undefined				based on casing dimensions given
Rock wool, at plant/CH U	6	kg	Undefined				estimate
Nickel, 99.5%, at plant/GLO U	1.5	kg	Undefined				estimate
Electronics for control units/RER S	0.5	kg	Undefined				estimate
Alkyd paint, white, 60% in H2O, at plant/RER U	0.25	kg	Undefined				estimate - powder coated paint unavailable
Synthetic rubber, at plant/RER U	0.25	kg	Undefined				estimate- feet, seals etc.
Sanitary ceramics, at regional storage/CH U	2.5	kg	Undefined				walls of furnace-only ceramic dataset available

Horizontal Furnace

Name: Horizontal Reactor

Image:

Comment: Very similar to that modelled for MWNT
**changes to datasets

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Steel, converter, low-alloyed, at plant/RER U	14	kg	Undefined				
Nickel, 99.5%, at plant/GLO U	1.28	kg	Undefined				
Silicon carbide, at plant/RER U	3.8	kg	Undefined				
Aluminium, production mix, cast alloy, at plant/RER U	1	kg	Undefined				
Rock wool, packed, at plant/CH U	7	kg	Undefined				DIFFERENT - used rockwool not the duct insulation modelling
Cable, connector for computer, without plugs, at plant/GLO U	3	m	Undefined				
Glass tube, borosilicate, at plant/DE U	2	kg	Undefined				
Furnace Large Controller_2013	1	p	Undefined				**new - 07/01/2013

Mechanical Stirrer

Name: Mechanical stirrer

Image:

Comment: Assumptions. Based on manufacturer supplied drawing. And likely material compositions

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Steel, low-alloyed, at plant/RER U	1	kg	Undefined				mostly steel construction casing material, fasteners etc.
CD-ROM/DVD-ROM drive, desktop computer, at plant/GLO U	1	p	Undefined				Mass of component = 0.9kg chosen this dataset since the motor, controller, casing complexity, operating voltage of 12v for most cd driveds however some run at 24V relate to 24v of stirrer motor. Torque similar. Missing- variable speed controller
Electronics for control units/RER U	0.05	kg	Undefined				Think much of electronic will be covered above, additional electronics added to account for heating operation.
Nickel, 99.5%, at plant/GLO U	0.20	kg	Undefined				heating element
Polypropylene injection moulding E	0.25	kg	Undefined				common plastic used in appliances, likely candidate
Aluminium, production mix, at plant/RER U	0.10	kg	Undefined				

Mass Flow Controller

Name: MFC Infrastructure

Image:

Comment:

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Glass fibre reinforced plastic, polyamide, injection moulding, at plant/RER U	0.096	kg	Undefined				
Stainless steel hot rolled coil, annealed & pickled, elec. arc furnace route, prod.	0.38	kg	Undefined				
Aluminium, production mix, cast alloy, at plant/RER U	0.07	kg	Undefined				
Flat glass, uncoated, at plant/RER S	0.019	kg	Undefined				
Brass, at plant/CH U	0.03	kg	Undefined				
Synthetic rubber, at plant/RER U	0.02	kg	Undefined				
CZ single crystalline silicon, electronics, at plant/RER U	0.0	kg	Undefined				the datasheet means silicon sealant not crystal - deducting this 20g amount , has approx >15% affect on certain impact categories
Polyvinylfluoride, at plant/US S	0.01	kg	Undefined				Nothing for FKM found, this used since it is a similar material containing fluoride, synthetic rubber had no fluorine content so this is included as a supplement.
Electronic component, unspecified, at plant/GLO U	2	g	Undefined				
Printed wiring board, surface mount, lead-containing surface, at plant/GLO U	5	cm2	Undefined				
Electronics for control units/RER U	10	g	Undefined				

Rotary Evaporator and Water Heating Bath

Name: Rotary Evaporator & Bath

Image

Comment: Data based on manufacturer brochure.
**new/amended datasets 07/01/2013

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Aluminium, production mix, cast alloy, at plant/RER U	7.5	kg	Undefined				housing
Steel, converter, chromium steel 18/8, at plant/RER U	4	kg	Undefined				
Polyethylene terephthalate, granulate, bottle grade, at plant/RER U	3	kg	Undefined				used PET because PBT unavailable - assumed similar
Synthetic rubber, at plant/RER U	0.1	kg	Undefined				
Glass tube, borosilicate, at plant/DE U	1	kg	Undefined				glassware, condenser
Electronics for control units/RER U	0.5	kg	Undefined				estimate by visual inspection
Copper wire, technology mix, consumption mix, at plant, cross section 1 mm² EU-	0.15	kg	Undefined				Electric motor windings

Sonicator Bath

Name: Sonicator_2013

Image

Comment: Total weight 1.4kg for 0.5litre unit

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Chromium steel 18/8, at plant/RER U	1.15	kg	Undefined				
Furnace Large Controller_2013	0.1	p	Undefined				**new 07/01/2013, good approximation of controller size comparison by insepction

Vacuum Pump

Name	Image	Comment
Vacuum Pump		

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Steel, low-alloyed, at plant/RER U	2.3	kg	Undefined				
Tetrafluoroethylene, at plant/RER U	2	kg	Undefined				
Synthetic rubber, at plant/RER U	0.5	kg	Undefined				
Fluorine, liquid, at plant/RER U	0.5	kg	Undefined				
Electronics for control units/RER U	0.2	kg	Undefined				
Copper wire, technology mix, consumption mix, at plant, cross section 1 mm² EU-	0.2	kg	Undefined				
Ferrite, at plant/GLO U	0.2	kg	Undefined				

Complete Modelled Synthesis: Example shown includes all above datasets, used for Catalyst Fe20 model.

Name: Cat_Fe_Synthesis

Image

Comment: Cradle-to-gate impacts 1 gram of Cat_Fe

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
a 20wt%Fe/SiO2	1/2.72 = 0.368	p					C
Methanol	0.368	p	Undefined				C
Silica [2 grams]	0.368	p	Undefined				C
Water Usage	0.368	p	Undefined				C
Hydrogen gas used - pretreat	0.368	p	Undefined				C
1. Mechanical Stirrer Elec (incl 4)	0.368	p	Undefined				E
2. Mechanical Stirrer Elec	0.368	p	Undefined				E
3. Mechanical Stirrer Elec	0.368	p	Undefined				E
5. Sonicator Elec	0.368	p	Undefined				E
6i. Rotional Evaporator	0.368	p	Undefined				E
6ii. Rotational Evaporator - Water Bath	0.368	p	Undefined				E
6iii. Rotational Evaporator - Pump	0.368	p	Undefined				E
7. Furnace	0.368	p	Undefined				E
8. H. Furnace - Ramp-up	0.368	p	Undefined				E
9. H. Furnace - Pre-treatment	0.368	p	Undefined				E
10. H. Furnace - 2nd ramp-up	0.368	p	Undefined				E
Mechanical stirrer	0.368*1.3699E-04 = 5.04E-5	p					I
Sonicator_2013	0.368*1.3699E-04 = 5.04E-5	p					I
Rotary Evaporator & Bath_2013	0.368*9.1324E-05 = 3.36E-5	p					I
Vacuum Pump	0.368*1.3699E-04 = 5.04E-5	p					I
Furnace 1100C_2013	0.368*2.2831E-05 = 8.4E-6	p					I
Horizontal Reactor_2013	0.368*5.4795E-05 = 2.02E-5	p					I
MFC Infrastructure_revised_2013	0.368*9.1324E-05 = 3.36E-5	p					I
(Insert line here)							

Modelled Catalyst Regeneration Dataset

Process:

- 50sccm of O_2 for 1 hour at elevated furnace temp, 500°C ~ double energy requirement for furnace temp of 300°C
- Catalyst activation phase under 50 sccm for 2 hours, furnace temp 300°C, see step 9 of catalyst testing.

Name: Catalyst Regeneration

Image

Comment:

Status: None

Materials/Assemblies	Amount	Unit	Distribution	SD^2 or 2*SMin		Max	Comment
9. H. Furnace - Pre-treatment	1	p	Undefined				
11. H. Furnace - Reaction	2	p	Undefined				
Hydrogen gas used - pretreat	1	p	Undefined				
Oxygen, liquid, at plant/RER S	0.1227	g	Undefined				
Horizontal Reactor_2013	5.4795E-5	p	Undefined				
MFC Infrastructure_revised_2013	9.1324E-5*2 = 0.000183	p					for both H2 and Oxygen runs
(Insert line here)							

Processes	Amount	Unit	Distribution	SD^2 or 2*SMin	Max	Comment
(Insert line here)						

Normalised Infrastructure Impacts

Title: Comparing product stages

Method: ReCiPe Midpoint (H) V1.05 / Europe ReCiPe H

Indicator: Normalisation

Impact category	Climate change	Ozone depletion	Human toxicity	Photochemical oxidant formation	Particulate matter formation	Ionising radiation	Terrestrial acidification	Freshwater eutrophication	Marine eutrophication	Terrestrial ecotoxicity	Freshwater ecotoxicity	Marine ecotoxicity	Agricultural land occupation	Urban land occupation	Natural land transformation	Water depletion	Metal depletion	Fossil depletion
Mechanical stirrer	2.17E-03	1.02E-04	1.61E-01	2.25E-03	7.71E-03	1.44E-03	1.21E-02	1.51E-01	1.75E-03	9.34E-04	1.30E-01	1.72E-01	1.45E-04	1.25E-03	2.37E-02	0.00E+00	3.77E-02	4.42E-03
Sonicator_2013	5.82E-04	1.86E-05	1.18E-02	4.15E-04	1.89E-03	2.72E-04	9.99E-04	1.18E-02	3.69E-04	2.10E-04	4.02E-02	5.52E-02	3.91E-05	2.35E-04	4.75E-03	0.00E+00	2.41E-02	1.19E-03
Rotary Evaporator & Bath_2013	5.84E-03	2.47E-04	1.50E-01	3.90E-03	1.19E-02	2.68E-03	8.94E-03	1.54E-01	3.38E-03	1.20E-03	2.25E-01	3.03E-01	4.06E-04	2.31E-03	6.85E-02	0.00E+00	1.03E-01	1.29E-02
Vacuum Pump	5.93E-02	8.57E-01	1.46E-01	2.40E-03	6.72E-03	2.52E-03	9.77E-03	8.82E-02	1.91E-03	5.84E-04	6.63E-02	8.86E-02	2.40E-04	8.33E-04	4.48E-02	0.00E+00	3.71E-02	8.08E-03
Furnace 1100C_2013	6.49E-03	1.82E-04	2.74E-01	8.44E-03	4.19E-02	1.98E-03	7.05E-02	2.48E-01	-1.86E-04	3.12E-03	2.88E-01	3.95E-01	4.32E-04	2.13E-03	7.07E-02	0.00E+00	5.56E-02	1.24E-02
Horizontal Reactor_2013	8.93E-03	3.45E-04	2.74E-01	9.65E-03	4.57E-02	4.93E-03	6.63E-02	2.95E-01	6.56E-03	3.83E-03	3.36E-01	4.73E-01	8.43E-04	3.22E-03	1.64E-01	0.00E+00	1.49E-01	2.03E-02
MFC Infrastructure_revised_2013	3.23E-04	1.07E-05	1.22E-02	2.10E-04	5.38E-04	1.00E-04	5.86E-04	1.06E-02	2.24E-04	6.50E-05	8.06E-03	1.11E-02	1.10E-05	8.21E-05	1.77E-03	0.00E+00	2.70E-03	5.79E-04

Renewable Hydrogen Dataset

Known outputs to technosphere. Products and co-products

Name	Amount	Unit	Quantity	Allocation	Waste type	Category	Comment
Hydrogen, RENEWABLE, liquid, membrane cell, at plant/RER U	1	kg	Mass	100 %	not defined	Chemicals\Gases	Europe
(Insert line here)							

Known outputs to technosphere. Avoided products

Name	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)							

Inputs

Known inputs from nature (resources)

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Water, unspecified natural origin/m3	in water	0.00088214	m3	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Water, cooling, unspecified natural origin/m3	in water	0.046429	m3	Lognormal	1.6			(2,5,3,1,4,5); estimate based on literature source
(Insert line here)								

Known inputs from technosphere (materials/fuels)

Name	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Sodium chloride, powder, at plant/RER U	0.8125	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Soda, powder, at plant/RER U	0.0053393	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Barite, at plant/RER U	0.001625	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Calcium chloride, CaCl2, at regional storage/CH U	0.0082643	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Hydrochloric acid, 30% in H2O, at plant/RER U	0.011607	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Sulphite, at plant/RER U	0.000046429	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Sodium hydroxide, 50% in H2O, production mix, at plant/RER U	0.0195	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Transport, lorry >16t, fleet average/RER U	0.10771	tkm	Lognormal	2.1			(4,5,n.a.,n.a.,n.a.,n.a.); Standard distances
Transport, freight, rail/RER U	0.00975	tkm	Lognormal	2.1			(4,5,n.a.,n.a.,n.a.,n.a.); Standard distances
Chemical plant, organics/RER/I U	0.00000000018571	p	Lognormal	3.8			(4,5,1,3,5,4); Estimation
Electricity, at wind power plant/RER U	1.29407142857142854	kWh	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
(Insert line here)							

Known inputs from technosphere (electricity/heat)

Name	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)							

Renewable Hydrogen Dataset (continued)

Emissions to air

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Hydrogen	high. pop.	0.00025536	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
Chlorine	high. pop.	0.000003714	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
Carbon dioxide, fossil	high. pop.	0.0014393	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Heat, waste	high. pop.	4.662142857	MJ	Lognormal	1.2			(1,3,1,1,1,5); Calculated (based on Electricity input)
(Insert line here)								

Emissions to water

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Chlorate	river	0.000975	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
Bromate	river	0.00012768	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
Chloride	river	0.0069643	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
Chlorinated solvents, unspecified	river	0.000000271	kg	Lognormal	3.1			(1,3,1,1,1,5); EC IPPC study 2002
Sulfate	river	0.0036679	kg	Lognormal	1.6			(1,3,1,1,1,5); EC IPPC study 2002
(Insert line here)								

Emissions to soil

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)								

Final waste flows

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)								

Non material emissions

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)								

Social issues

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)								

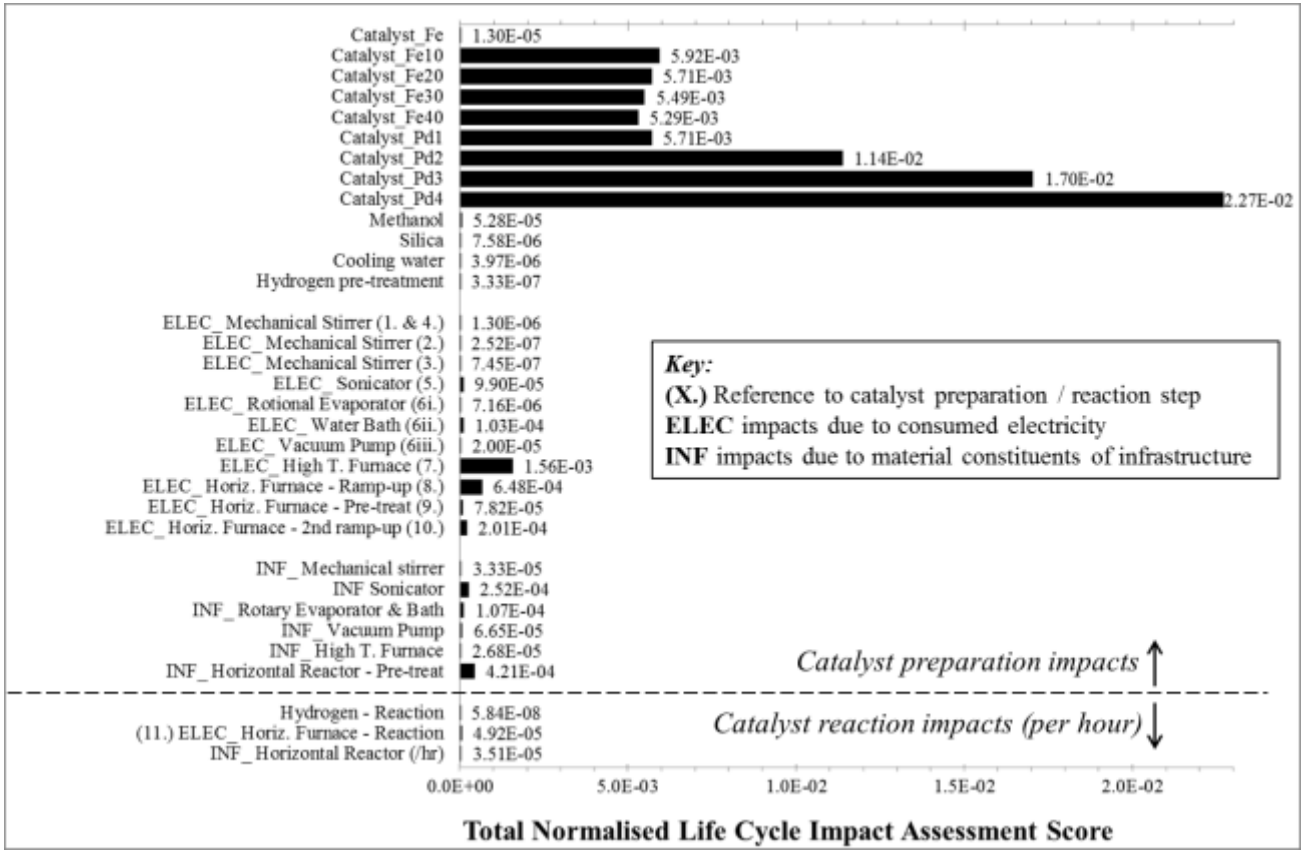
Economic issues

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
(Insert line here)								

Known outputs to technosphere. Waste and emissions to treatment

Name	Amount	Unit	Distribution	SD^2 or 2*S	Min	Max	Comment
Disposal, sludge, NaCl electrolysis, 0% water, to residual material landfill/CH U	0.0071036	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
Disposal, paper, 11.2% water, to sanitary landfill/CH U	0.00027857	kg	Lognormal	1.2			(1,3,1,1,1,5); EC IPPC study 2002
(Insert line here)							

LCIA for all Catalyst steps.



LCIA contributions per gram of catalyst formed. Catalyst reaction impacts are measured per hour of reaction. Total sum of the 18 ReCiPe midpoint score values.

References:

1. Ecoinvent Database v2.2, May 2010 edn.