Supplementary Materials

The role of hydrogen in the ecological benefits of Ultra Low Sulphur Diesel production and use: an LCA benchmark

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Table S1. Utilities in the HDT process. Top: feed with variable S content converted into S-free naphtha and diesel with a constant S content (38 ppm wt). Bottom: feed with constant S content (1.57 wt%) used to produce S-free naphtha and diesel with variable S content. Data from Wu et al. [20].

S in feed	S in diesel	Feed	Diesel	Naphtha	Make-up H_2	HP-steam (cycle H_2 compressor)	Fuel gas (preheating HDT feed)	Electricity	Avoided SO_2
(%)	(ppm)	(kg/h)	(kg/h)	(kg/h)	(Nm^3/h)	(kW)	(kW)	(kW)	(kg/h)
1.3	38.6	380,900	334,000	38,100	30,419	1829	7236	6002.1	9878
1.4	38,5	380,900	334,000	38,100	31,651	1829	6720	6098.7	10,639
1.5	38	380,900	334,000	38,100	32,906	1829	6517	6196.8	11,402
1.5711	38.2	380,900	334,000	38,100	33,779	1829	6315	6266.7	11,943
1.7	38.3	380,900	334,000	38,100	35,392	1829	5760	6392.5	12,925
1.8	38.9	380,900	334,000	38,100	36,624	1829	5518	6489.2	13,686
1.5711	7.4	380,900	334,000	38,100	33,802	2679	9160	6481.9	11,964
1.5711	38.2	380,900	334,000	38,100	33,779	1829	6315	6266.7	11,943
1.5711	75.2	380,900	334,000	38,100	33,690	1627	4758	6204.2	11,918
1.5711	104.1	380,900	334,000	38,100	33,667	1394	4193	6148.5	11,899
1.5711	132.6	380,900	334,000	38,100	33,600	1241	3619	6087.7	11,880
1.5711	167.3	380,900	334,000	38,100	33,555	1070	3249	6030.1	11,857
1.5711	191.7	380,900	334,000	38,100	33,510	1070	3062	6026.60	11,841
1.5711	228.3	380,900	334,000	38,100	33,443	1070	2875	6021.30	11,816
1.5711	266.3	380,900	334,000	38,100	33,376	1070	2689	6016.30	11,791
1.5711	318.6	380,900	334,000	38,100	33,286	1070	2589	6009.30	11,756

Table S2. Utilities and eco-costs of Amine Treating and Sulphur Recovery processes. Data for consumption by Barthe et al. [12].

Process	Utility or Emissions	Consumption/ Emissions	Eco-costs (€//kg avoided SO_2)		
			EU grid electricity	Windpower	Hydropower
Amine treating	Electricity	0.037–0.043 (kWh/kg avoided SO_2)	0.0038–0.0044	0.00021–0.00024	0.00006–0.00007
	Steam	0.80–1.59 (kg/kg avoided SO_2)	0.0336–0.0672	0.0336–0.0672	0.0336–0.0672
	Cooling water	0.01–0.02 (m^3/kg avoided SO_2)	0.0104–0.0145	0.0104–0.0145	0.0104–0.0145
Sulphur recovery Unit	Electricity	0.030–0.038 (kWh/kg avoided) SO_2)	0.0031–0.0039	0.00017–0.00022	0.00005–0.00006
	Fuel	0.013–0.021 (Nm^3/kg avoided SO_2)	0.0008–0.0013	0.0008–0.0013	0.0008–0.0013
	Cooling water	0–0.010 (m^3/kg avoided SO_2)	0–0.0078	0–0.0078	0–0.0078
	SO_2 emissions	0.001 (kg/kg avoided SO_2)	0.0088	0.0088	0.0088

Table S3. SMR + CCS cases: consumption, production and CO_2 emissions. Data from IEAGHG Technical Report 2017-02, Table 2 therein [16].

CASE	Amount	Base case—SMR without CCS	2B—SMR + CO_2 capture from PSA tail gas (cryogenic and membrane separation)	3—SMR + CO_2 capture from SMR flue gas (MEA absorption)
Natural gas consumption	kWh/kg H_2	43.89	43.79	48.22
H_2 production	kg/h	8994	8994	8994
Gross electricity produced from COGEN plant	kWh/kg H_2	1.28	1.22	1.30
Electricity consumed for H_2 plant	kWh/kg H_2	(0.14)	(0.14)	(0.15)
Electricity consumed for COGEN auxiliaries, utilities, BoP	kWh/kg H_2	(0.04)	(0.06)	(0.19)
Electricity consumed for CO_2 capture	kWh/kg H_2	0	(1.00)	(0.22)
Electricity for CO_2 compression and drying	kWh/kg H_2	0	see Note	(0.70)
Electricity export to grid	kWh/kg H_2	1.10	0.03	0.05
CO_2 emitted	kg/kg H_2	9.09	4.24	1.00
CO_2 captured	kg/kg H_2	0	4.82	8.99
CO_2 capture rate (case specific)	%	0	53	90
CO_2 capture rate (as compared to base case)	%	0	53	89
MEA (monoethanolamine) [a]	kg/kg H_2	0	0	0.0026

Note: CO_2 compression and drying included in the CO_2 capture plant

Value within brackets are for consumption figures.

a: MEA consumption from Nexant "Carbon Capture and Sequestration", PERP2012S1: 0.294 kg MEA/ton CO_2 captured.

Table S4. LCI and eco-costs for hydrogen from water alkaline electrolysis (AEL). The entire AEL life cycle corresponds to 19,588,000 kgH_2 = (20y)x(8300h/y)x(118kg H_2/h). Eco-costs are calculated for two electricity scenarios: windmill and hydropower. Quantities of materials from Koj et al. [28].

Section	Item	Ecoinvent	Amount (for AEL life cycle)		Eco-costs (€/kg H_2)
Cell stack Framework	Copper	56% Copper {RER} production, primary + 44% Copper {RER} treatment of scrap by electrolytic refining	t	2	0.000302
	Unalloyed steel	Steel, unalloyed {GLO} market	t	200	0.005419
Cell Stack Construction	Nickel	Nickel from Nickel Institute 2012	t	19	0.020591
	Aluminium	Aluminium, primary, ingot {IAI Area, EU27 & EFTA} market	kg	450	0.000084
	Calendered rigid plastic	Polypropylene granulate (PP), production mix, at plant RER w/t oil eco-cost	kg	780	0.000045
	Polytetrafluoroethylene	Idematapp2018 PTFE (Teflon, Polytetrafluoroethylene), estimate *	kg	78	0.000006
	Acrylonitrile butadiene styrene	Acrylonitrile-butadiene-styrene granulate (ABS), production mix, at plant RER with oil eco-cost	kg	160	0.000012
	Polyphenylene sulfide	Polyphenylene sulfide {GLO} market with oil eco-costs	kg	340	0.000039
	Polysulfones	Polysulfone {GLO} market with oil eco-costs	kg	260	0.000023
	N-Methyl-2-pyrrolidone	N-methyl-2-pyrrolidone {RER} production with oil eco-cost	t	1,3	0.000127
	Aniline	Aniline {GLO} market	kg	49	0.000003
	Acetic anhydride	Acetic acid, without water, in 98% solution state {GLO} market with oil eco-cost	kg	54	0.000002
	Terephthalic acid	Purified terephthalic acid {GLO} market	kg	88	0.000002
	Nitric acid	Nitric acid, without water, in 50% solution state {GLO} market	kg	33	0.000001
	Hydrochloric acid	Hydrochloric acid, without water, in 30% solution state {RER} market	kg	130	0.000001
	Graphite	Anode, graphite, for lithium-ion battery {GLO} market	kg	430	0.000084
	Lubricating oil	Lubricating oil {GLO market	kg	0.48	0.000000
	Zirconium oxide	Zirconium oxide {GLO} market	t	1.1	0.001029
	Carbon monoxide	Carbon monoxide {RER} market	kg	150	0.000003
	Decarbonized water	Water, decarbonised, at user {GLO} market	t	11	0.000000
	Deionized water	Water, deionised, from tap water, at user {Europe without Switzerland} market for water, deionised, from tap water, at user	t	86	0.000003
	Electricity	Electricity, high voltage {Europe without Switzerland}market group	GJ	36	0.000053
	Heat	Heat, district or industrial, natural gas {RER} market group	GJ	88	0.000032
	Steam	Heat, district or industrial, natural gas {RER} market group	MJ	700	0.000000
	Industrial machine production		kg	0.16	
	Plaster mixing		kg	780	
Plant construction	Steel for heat exchanger	Steel, unalloyed {GLO} market	kg	3900	0.020591
	Steel for tank KOH		kg	4000	
	Water tank		L	31,200	
	Steel for gas separator		kg	4970	

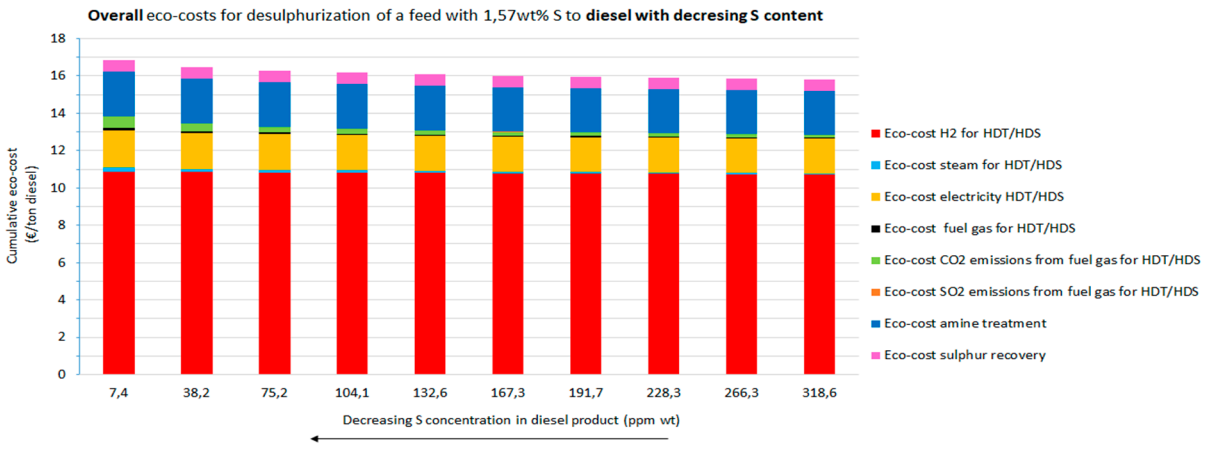
	Steel KOH filter		kg	145		
	Inverter unit (2.5 MW <5000kg)	Transformer, low voltage use {GLO} market	piece	1	0.001256	
		Subtotal 1 (construction)			**0.02956**	
Electricity					Windmill	Hydro
Electricity (operation)	Electricity	Electricity, high voltage {NO} electricity production, hydro, reservoir, alpine region	MJ	352,5840,000	0.287444	0.080945
Other (operation)	Deionized water	Water, deionised, from tap water, at user {RoW} market for water, deionised, from tap water, at user	kg	195,880,000	0.012328	
	Nitrogen	Nitrogen, liquid {RER}market	g	5,680,520	0.000017	
	Potassium hydroxide	Potassium hydroxide {GLO}market	g	37,217,200	0.000861	
	Steam	Steam, in chemical industry {RER} production	kg	2,154,680	0.004639	
		Subtotal 2 (operation)			**0.30529**	**0.09879**
		TOTAL			**0.33485**	**0.12836**

Table S5. Background LCI data.

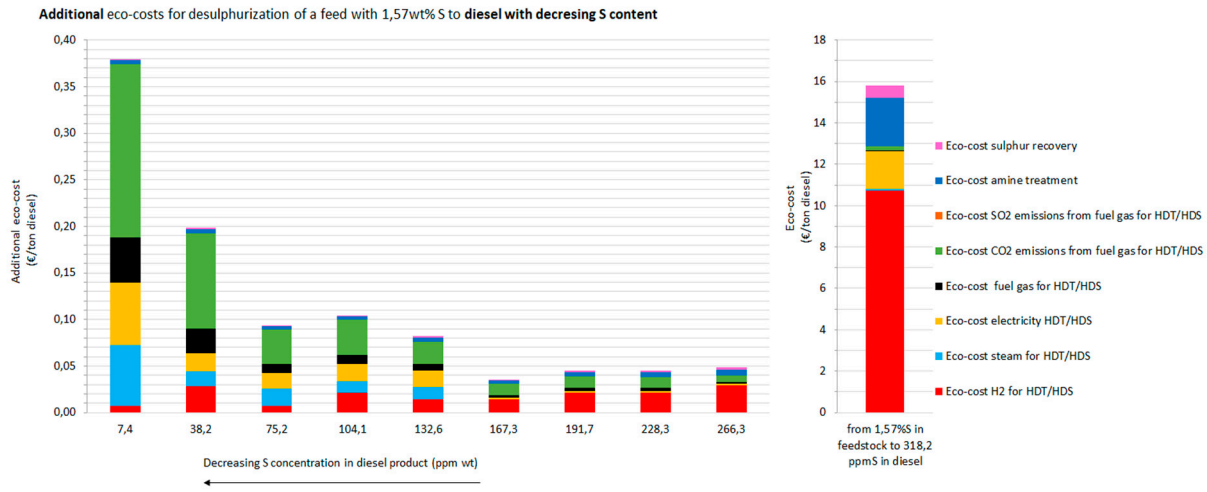
Unit	**Ecoinvent**	**Eco-cost**					**Damage**		
		Total	**Human health**	**Eco-toxicity**	**Resources**	**C-footprint**	**Human health**	**Eco-system**	**Resources availability**
		(€)	(€)	(€)	(€)	(€)	(DALY)	(Species x year)	(US $2013)
MJ	Heat, district or industrial, natural gas {RER} market group	0.0071	0.0001	0.0004	0.0001	0.0066	8.9×10^{-7}	1.5×10^{-9}	7.9×10^{-3}
m^3	Natural gas, high pressure {Europe without Switzerland} market group	0.061	0.003	0.011	0.001	0.045	6.1×10^{-7}	1.5×10^{-9}	3.6×10^{-1}
MJ	Electricity, high voltage {Europe without Switzerland} market group	0.029	0.001	0.006	0.007	0.014	2.5×10^{-7}	5.7×10^{-10}	4.7×10^{-3}
kg	Water, deionised, from tap water, at user {Europe without Switzerland} market for water, deionised, from tap water, at user	0.001	0	0	0.001	0	4.5×10^{-9}	1.8×10^{-11}	5.1×10^{-5}
kg	Steam, in chemical industry {RER} production	0.042	0.002	0.007	0.001	0.033	4×10^{-7}	1×10^{-9}	3×10^{-2}
kg	Monoethanolamine {GLO}| market	0.589	0.049	0.159	0.041	0.340	5.5×10^{-6}	1.2×10^{-8}	5.5×10^{-1}
MJ	Electricity, high voltage {DK}| electricity production, wind, 1-3MW turbine, offshore	0.00160	0.0004	0.0002	0.0004	0.0005	1.2×10^{-8}	2×10^{-11}	3.2×10^{-4}
MJ	Electricity, high voltage {NO}| electricity production, hydro, reservoir, alpine region	0.00045	0.0001	0.0001	0.0001	0.0002	2.2×10^{-8}	1.2×10^{-10}	9.9×10^{-5}
kg	SO2 emission			8.75			1.8×10^{-4}	2.1×10^{-7}	
kg	CO_2 emissions					0.116	9.3×10^{-7}	2.8×10^{-9}	

Table S6. 'Overall' 'eco-cost production' and 'avoided eco-cost' for the desulphurization of a feedstock with 1.57 wt% S to diesel with variable S content.

SCENARIO: Variable S content in diesel, H_2 from SMR without CCS											
S in feed	(%)	**1.5711**									
S in diesel	(ppm wt)	**7.4**	**38.2**	**75.2**	**104.1**	**132.6**	**167,3**	**191.7**	**228.3**	**266.3**	**318.6**
H_2 for HDT/HDS	(€/ton diesel)	10.87	10.9	10.8	10.8	10.8	10.8	10.8	10.8	10.7	10.7
HP steam	(€/ton diesel)	0.21	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
electricity	(€/ton diesel)	2	1.9	1.9	1.9	1.9	1.9	1.9	1.9	1.9	1.9
fuel gas preheating for HDT	(€/ton diesel)	0.16	0.1	0.1	0.1	0.1	0.1	0.1	0	0.0	0
CO_2 from combustion of fuel gas for preheating for HDT	(€/ton diesel)	0.60	0.4	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2
SO_2 from combustion of fuel gas for HDT	(€/ton diesel)	0	0	0	0	0	0	0	0	0	0
HDT (H_2 excluded)	(€/ton diesel)	2.97	2.6	2.4	2.4	2.3	2.2	2.2	2.2	2.2	2.2
Amine treating (average)	(€/ton diesel)	2.40	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4
SRU (average)	(€/ton diesel)	0.62	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
Total 'eco-cost production'	(€/ton diesel)	**19.82**	**19.1**	**18.7**	**18.5**	**18.4**	**18.2**	**18.2**	**18.1**	**18**	**18**
Total 'avoided eco-cost'	(€/ton diesel)	**313.42**	**312.9**	**312.2**	**311.7**	**311.2**	**310.6**	**310.2**	**309.6**	**308.9**	**308**
H_2 'eco-cost production' (as percent of total 'eco-cost production')	(%)	**63.6**	**65.3**	**66**	**66.4**	**66.8**	**67.1**	**67.1**	**67.2**	**67.2**	**67.2**
'Avoided eco-cost'/'Eco-cost production'	(€/€)	**18.3**	**18.8**	**19**	**19.1**	**19.2**	**19.3**	**19.3**	**19.3**	**19.3**	**19.4**



(a)

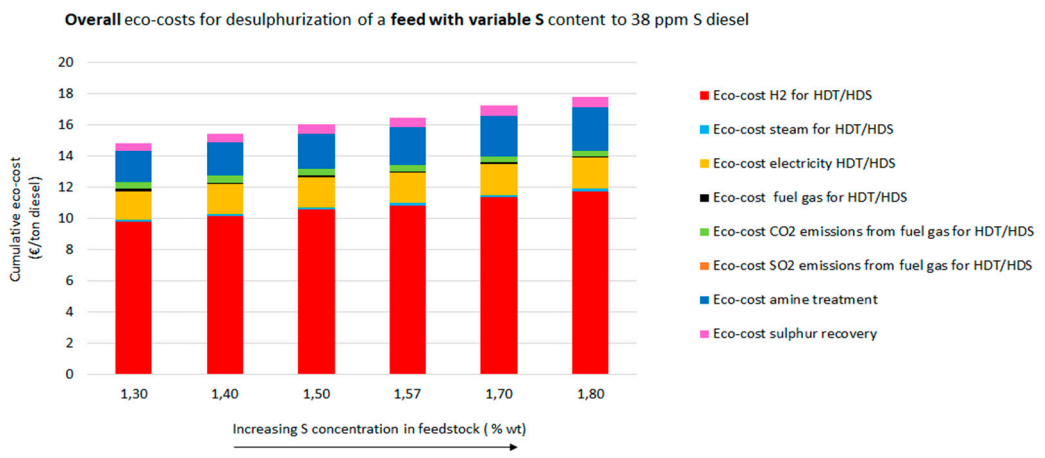


(b)

Figure S1. Desulphurization of a feedstock with 1.57wt% S to diesel with variable S content using H_2 from SMR: 'Overall' 'eco-cost of production' **(a)** and 'additional' 'eco-cost of production' **(b)**.

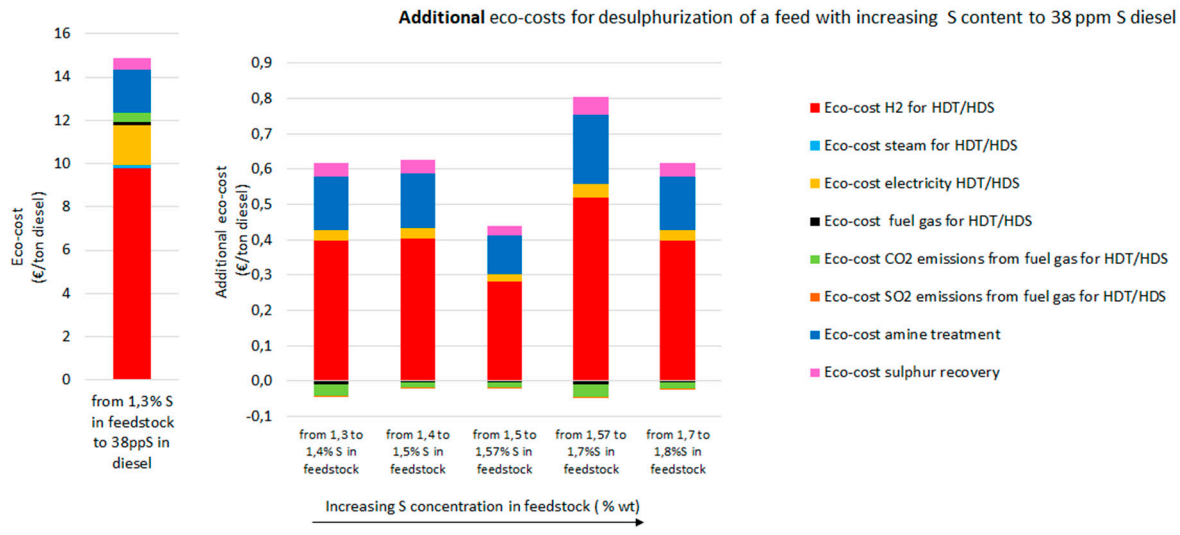
Table S8. 'Overall' 'eco-cost of production' and 'avoided eco-cost' for the desulphurization of a feedstock with variable S content to a 38 ppm S diesel.

SCENARIO: Variable S content in feedstock; H_2 from SMR without CCS							
S in feed	(%)	1.30	1.40	1.50	1.57	1.70	1.80
S in diesel	(ppm wt)	38.6	38.5	38	38.2	38.3	38.9
H_2 for HDT/HDS	(€/ton diesel)	9.78	10.18	10.58	10.86	11.38	11.78
HP steam	(€/ton diesel)	0.14	0.14	0.14	0.14	0.14	0.14
electricity	(€/ton diesel)	1.86	1.89	1.92	1.94	1.98	2.01
fuel gas preheating for HDT	(€/ton diesel)	0.13	0.12	0.11	0.11	0.10	0.10
CO_2 from combustion of fuel gas for preheating for HDT	(€/ton diesel)	0.47	0.44	0.43	0.41	0.38	0.36
SO_2 from combustion of fuel gas for HDT	(€/ton diesel)	0	0	0	0	0	0
HDT (H_2 excluded)	(€/ton diesel)	2.59	2.58	2.60	2.60	2.59	2.60
Amine treating (average)	(€/ton diesel)	1.98	2.13	2.29	2.40	2.59	2.75
SRU (average)	(€/ton diesel)	0.51	0.55	0.59	0.61	0.67	0.70
Total 'eco-cost production'	(€/ton diesel)	**14.87**	**15.44**	**16.05**	**1647**	**17.23**	**17.83**
'Avoided eco-cost'	(€/ton diesel)	**258.77**	**278.73**	**298.70**	**312.88**	**338.60**	**358.55**
H_2 'eco-cost production' (% of total 'eco-cost production')	(%)	**65.8**	**65.9**	**65.9**	**65.9.**	**66**	**66.1**
'Avoided eco-cost'/ 'Eco-cost production'	(€/€)	**17.4**	**18.1**	**18.6**	**19**	**19.7**	**20.1**



(a)

Figure S2. *Cont.*



(b)

Figure S2. Desulphurization of a feedstock with variable S content to diesel with 38 ppm S using H_2 from SMR: 'Overall' 'eco-cost of production' **(a)** and 'additional' 'eco-cost of production' **(b)**.