1 Supplementary information

1.1 Simulation results

Table 1: Main mass and energy flows as a results of the process modelling (NEC: *N*-ethylcarbazole, DBT: dibenzyltoluene, AB: 1,2-dihydro-1,2-azaborine, FA: formic acid, MET: methanol, NAP: naphthalene, TOL: toluene, CGH_2: Compressed Hydrogen Gas)

	NEC		DBT		AB		FA		MET		NAP	
De-hydrogenation Covering	Burner	Waste heat	Burner	Waste heat	Burner	Waste heat	Burner	Waste heat	Burner	Waste heat	Burner	Waste heat
	Mass flow [kg/h]											
Hydrogen input	39.6	30.0	40.1	30.0	34.2	30.0	34.8	30.0	33.0	30.0	41.9	30.0
Hydrogen burner	9.6	0.0	10.3	0.0	4.1	0.0	4.7	0.0	2.9	0.0	11.8	0.0
Hydrogen fuel cell	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
H_0LOHC	639.4	484.8	605.7	450.9	469.2	412.6	758.9	654.9	238.0	218.5	532.7	381.9
	Energy flow [kW]											
Electrolysis	1,915.2	1,452.2	1,950.8	1,452.2	1,651.9	1,452.2	1,680.9	1,452.2	1,590.7	1,452.1	2,025.6	1,452.3
Hydrogenation	-261.2	-198.1	-329.6	-246.5	-138.5	-121.6	-90.3	-86.3	-89.4	-83.0	-390.0	-286.5
De-hydrogenation	323.5	212.1	348.4	259.4	139.3	122.5	159.8	126.0	96.8	88.4	400.5	287.2
Hydrogen purification	0.0	0.0	0.0	0.0	107.0	94.1	198.1	170.8	135.3	123.5	124.9	89.6
H_2O-pump	1.8	1.2	1.6	1.2	1.4	1.2	1.4	1.2	1.4	1.2	1.9	1.2
Compressors	-	-	-	-	-	-	132.4	121.2	34.0	31.1	0	0
Blower	12.3	9.1	12.5	9.1	10.4	9.1	10.6	9.1	10.0	9.1	13.0	9.1
LOHC-pump	2.4	1.8	2.5	1.8	5.8	5.0	42.5	38.0	-	-	5.6	4.0
PSA	-	-	-	-	107.0	94.1	198.1	170.8	135.3	123.5	124.9	89.6
Distillation	-	-	-	-	-	-	8,8850.1	7873.8	-	-	-	-

	TOL		CGH_2
De-hydrogenation Covering	Burner	Waste heat	-
	Mass flows [kg/h]		
Hydrogen input	42.0	30.0	30.0
Hydrogen burner	12.0	0.0	-
Hydrogen fuel cell	30.0	30.0	30.0
H_0LOHC	640.2	457.6	-
	Energy flows [kW]		
Electrolysis	2,031.9	1,452.3	1,452.1
Hydrogenation	-396.3	-283.2	-
De-hydrogenation	405.0	295.9	-
Hydrogen purification	130.6	93.4	-
H_2O-pump	1.5	1.2	1.2
Compressors	0	0	32.8[a]
Blower	13.1	9.1	9.1
LOHC-pump	1.1	1.2	-
PSA	130.6	93.4	-
CO_2-Absorption	-	-	-

[a] H_2-compressor

1.2 Base and design information of the equipment

Table 2: Base and design information for the equipment cost calculation

Unit	Overall ratio factor	Base Capacity	Unit	Design Capacity	Base Cost [€]	Scaling Factor	No. Units	Base Year	Ref.
Hydrogen burner	4.60	50.7	MW	$\dot{Q}_{burner}$	3,850,000	0.83	1	2002	[1]
Blower	4.60	26	m^3/s	$\dot{V}_{blower}$	16,830	0.57	2 (1)	2002	[1]
PSA Unit	1.83	168.75	$kg_{H2,feed}/h$	$\dot{m}_{PSA}$	205,000,000	1.00	1	2013	[2]
Compressor	4.60	6	MW	$P_{compressor}$	1,120,000	0.68	1	2002	[1]
Pump	4.60	1	m^3/s	$\dot{V}_{pump}$	17,820	0.36	2	2002	[1]
Electrolysis	1.83	1	kW	$P_{electrolysis}$	760	1.00	1	2016	[3]
Fuel cell	1.83	1	kW	$P_{fuel\ cell}$	3,010	1.00	1	2015	[4]
H_2-compressor	1.83	1	kW	$P_{H2,compressor}$	2,500	1.00	1	2006	[5]
H_2-pressure tank	1.83	1	kg_{H2}	m_{H2}	380[a]/930[b]	1.00	1	2014	[6]
LOHC-tank	4.60	1	m^3	V_{LOHC}	193	1.00	2	2014	[7]
Hydrogenation	1.83	30	kg/h	$\dot{m}_{H2,out}$	Eq. (5)	0.60	1	2017	[7, 8]
De-hydrogenation	1.83	30	kg/h	$\dot{m}_{H2,out}$	Eq. (6)	0.60	1	2017	[7, 8]
Cavern	1.83	500,000	m^3	V_{H2}	3,800,000	0.28	1	2013	[9]
Distillation	4.60	104.9	kg/h	$\dot{m}_{in}$	50,000	0.70	2	2006	[10]

[a] 200 bar, [b] 700 bar

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