Supplementary Materials: CO_2 Hydrogenation to Methanol by a Liquid-Phase Process with Alcoholic Solvents: A Techno-Economic Analysis

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Table S1. Stream table for the gas-phase CO_2 hydrogenation to methanol process.

Stream		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Temperature	C	20	78	20	113	30	126	30	128	30	97	44	215	274	274	74	274	124
Pressure	bar	30	51	1	3	3	8	8	25	24	51	51	50	50	50	49	50	48
Molar Vapor Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Molar Liquid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	kmol/h	265	265	88	88	88	88	88	88	88	88	2223	2223	2078	1413	1413	665	665
CO_2	kmol/h	0	0	88	88	88	88	88	88	88	88	372	372	296	201	201	95	95
CO	kmol/h	0	0	0	0	0	0	0	0	0	0	99	99	102	69	69	33	33
Methanol	kmol/h	0	0	0	0	0	0	0	0	0	0	8	8	80	54	54	26	26
Hydrogen	kmol/h	265	265	0	0	0	0	0	0	0	0	1743	1743	1523	1035	1035	487	487
Water	kmol/h	0	0	0	0	0	0	0	0	0	0	2	2	77	52	52	25	25
Mass Flow	kg/h	533	533	3882	3882	3882	3882	3882	3882	3882	3882	22614	22614	22614	15377	15377	7236	7236
CO_2	kg/h	0	0	3882	3882	3882	3882	3882	3882	3882	3882	16095	16095	12773	8686	8686	4087	4087
CO	kg/h	0	0	0	0	0	0	0	0	0	0	2751	2751	2834	1927	1927	907	907
Methanol	kg/h	0	0	0	0	0	0	0	0	0	0	214	214	2538	1726	1726	812	812
Hydrogen	kg/h	533	533	0	0	0	0	0	0	0	0	3529	3529	3085	2098	2098	987	987
Water	kg/h	0	0	0	0	0	0	0	0	0	0	25	25	1384	941	941	443	443
Volume Flow	l/min	3650	2596	35641	15654	13058	5727	4341	1918	1330	786	19211	30568	32010	21767	13294	10243	7575

Table S1. (cont.).

Stream		18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
Temperature	C	67	72	35	35	35	35	37	35	29	29	29	81	69	104	35	35	35
Pressure	bar	47	47	47	47	47	47	51	50	1	1	1	1	1	1	1	1	1

Molar Vapor Fraction		1	1	1	1	1	1	1	0	0	1	0	0	1	0	0	0	1
Molar Liquid Fraction		0	0	0	0	0	0	0	1	1	0	1	1	0	1	1	1	0
Mole Flow	kmol/h	665	2078	2078	1924	54	1870	1870	154	154	7	147	147	71	76	71	71	0
CO_2	kmol/h	95	296	296	292	8	283	283	5	5	4	0	0	0	0	0	0	0
CO	kmol/h	33	102	102	102	3	99	99	0	0	0	0	0	0	0	0	0	0
Methanol	kmol/h	26	80	80	8	0	8	8	72	72	1	71	71	71	0	71	71	0
Hydrogen	kmol/h	487	1523	1523	1521	43	1478	1478	2	2	2	0	0	0	0	0	0	0
Water	kmol/h	25	77	77	2	0	2	2	75	75	0	75	75	0	75	0	0	0
Mass Flow	kg/h	7236	22614	22614	18713	514	18199	18199	3901	3901	232	3668	3668	2298	1371	2293	2290	3
CO_2	kg/h	4087	12773	12773	12558	345	12213	12213	215	215	198	16	16	16	0	16	14	2
CO	kg/h	907	2834	2834	2829	78	2751	2751	5	5	5	0	0	0	0	0	0	0
Methanol	kg/h	812	2538	2538	220	6	214	214	2318	2318	23	2295	2295	2280	15	2275	2275	1
Hydrogen	kg/h	987	3085	3085	3081	85	2996	2996	4	4	4	0	0	0	0	0	0	0
Water	kg/h	443	1384	1384	25	1	25	25	1359	1359	3	1356	1356	1	1355	1	1	0
Volume Flow	l/min	6275	19955	17443	16475	461	16015	15811	99	2456	2461	72	21374	27766	25	73	49	24

Table S2. Stream table for the liquid-phase CO_2 hydrogenation to methanol process with 2-butanol solvent.

Stream		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**
Temperature	C	20	80	20	113	30	126	30	128	30	99	62	142	180	180	172	161	149	118	35	35	35	35
Pressure	bar	30	52	1	3	3	8	8	25	24	52	52	51	50	50	49	48	47	46	45	45	45	45

Molar Vapor Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Molar Liquid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	kmol/h	265	265	88	88	88	88	88	88	88	88	1195	1195	1195	1388	1388	1388	1388	1388	1388	851	842	9
CO_2	kmol/h	0	0	88	88	88	88	88	88	88	88	119	119	119	39	39	39	39	39	39	31	31	0
CO	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0
Methanol	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	81	81	81	81	81	81	1	1	0
Hydrogen	kmol/h	265	265	0	0	0	0	0	0	0	0	1072	1072	1072	838	838	838	838	838	838	816	808	8
Water	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	144	144	144	144	144	144	1	1	0
2-Butanol	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	285	285	285	285	285	285	1	1	0
Mass Flows	kg/h	533	533	3882	3882	3882	3882	3882	3882	3882	3882	7533	7533	7533	29790	29790	29790	29790	29791	29791	3149	3118	31
CO_2	kg/h	0	0	3882	3882	3882	3882	3882	3882	3882	3882	5249	5249	5249	1736	1736	1736	1736	1736	1736	1381	1367	14
CO	kg/h	0	0	0	0	0	0	0	0	0	0	22	22	22	23	23	23	23	23	23	22	22	0
Methanol	kg/h	0	0	0	0	0	0	0	0	0	0	32	32	32	2600	2600	2600	2600	2600	2600	33	32	0
Hydrogen	kg/h	533	533	0	0	0	0	0	0	0	0	2162	2162	2162	1689	1689	1689	1689	1689	1689	1645	1628	16
Water	kg/h	0	0	0	0	0	0	0	0	0	0	14	14	14	2590	2590	2590	2590	2590	2590	14	14	0
2-Butanol	kg/h	0	0	0	0	0	0	0	0	0	0	54	54	54	21153	21153	21153	21153	21153	21153	55	54	1
Volume Flow	l/min	3650	2563	35641	15654	13058	5727	4341	1918	1330	775	10855	13748	15288	16504	15831	14810	13888	11874	8891	8232	8150	82

Table S2. (cont.).

Stream		**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**
Temperature	C	53	35	80	82	89	110	62	91	35	35	35	96	96	96	96	96	92	20	91	84	134	180

Pressure	bar	52	45	44	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	52	51	50
Molar Vapor Fraction		1.0	0.0	0.0	0.1	1.0	0.0	1.0	0.0	0.3	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Molar Liquid Fraction		0.0	1.0	1.0	0.9	0.0	1.0	0.0	1.0	0.7	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mole Flow	kmol/h	842	538	538	538	325	212	105	221	105	73	32	81	139	352	4	348	348	4	352	352	352	352
CO_2	kmol/h	31	8	8	8	8	0	8	0	8	0	8	0	0	0	0	0	0	0	0	0	0	0
CO	kmol/h	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	kmol/h	1	80	80	80	80	0	80	0	80	72	8	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	kmol/h	808	22	22	22	17	5	17	0	17	0	17	0	0	5	0	5	5	0	5	5	5	5
Water	kmol/h	1	143	143	143	143	0	0	143	0	0	0	79	64	64	1	63	63	0	63	63	63	63
2-Butanol	kmol/h	1	285	285	285	77	207	0	77	0	0	0	2	75	283	3	280	280	4	284	284	284	284
Mass Flow	kg/h	3118	26641	26641	26641	11259	15382	2946	8313	2946	2329	616	1574	6739	22121	221	21900	21900	296	22197	22197	22197	22197
CO_2	kg/h	1367	355	355	355	355	0	355	0	355	18	337	0	0	0	0	0	0	0	0	0	0	0
CO	kg/h	22	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	kg/h	32	2567	2567	2567	2567	0	2557	11	2557	2311	245	2	8	8	0	8	8	0	8	8	8	8
Hydrogen	kg/h	1628	44	44	44	34	10	34	0	34	0	34	0	0	10	0	10	10	0	10	10	10	10
Water	kg/h	14	2576	2576	2576	2576	0	0	2576	0	0	0	1429	1147	1147	11	1135	1135	0	1135	1135	1135	1135
2-Butanol	kg/h	54	21098	21098	21098	5726	15372	0	5726	0	0	0	142	5584	20956	210	20746	20746	296	21043	21043	21043	21043
Volume Flow	l/min	7500	658	750	15679	115013	368	40099	175	11717	50	11667	1699	147	6915	69	6846	496	6	502	570	624	708

Table S3. Stream table for the liquid-phase CO_2 hydrogenation to methanol process with 1-butanol solvent.

Stream		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**
Temperature	C	20	80	20	113	30	126	30	128	30	99	63	139	180	180	169	159	152	104	35	35	35	35
Pressure	bar	30	52	1	3	3	8	8	25	24	52	52	51	50	50	49	48	47	46	45	45	45	45
Molar Vapor Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Molar Liquid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	kmol/h	265	265	88	88	88	88	88	88	88	88	1057	1057	1057	1049	1049	1049	1049	1049	1049	711	704	7
CO_2	kmol/h	0	0	88	88	88	88	88	88	88	88	119	119	119	36	36	36	36	36	36	31	30	0
CO	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0
Methanol	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	84	84	84	84	84	84	1	1	0
Hydrogen	kmol/h	265	265	0	0	0	0	0	0	0	0	935	935	935	689	689	689	689	689	689	677	670	7
Water	kmol/h	0	0	0	0	0	0	0	0	0	0	1	1	1	106	106	106	106	106	106	1	1	0
1-Butanol	kmol/h	0	0	0	0	0	0	0	0	0	0	0	0	0	133	133	133	133	133	133	0	0	0
Mass Flow	kg/h	533	533	3882	3882	3882	3882	3882	3882	3882	3882	7199	7199	7199	17461	17461	17461	17461	17461	17461	2812	2784	28
CO_2	kg/h	0	0	3882	3882	3882	3882	3882	3882	3882	3882	5221	5221	5221	1594	1594	1594	1594	1594	1594	1353	1339	14
CO	kg/h	0	0	0	0	0	0	0	0	0	0	21	21	21	22	22	22	22	22	22	22	21	0
Methanol	kg/h	0	0	0	0	0	0	0	0	0	0	43	43	44	2698	2698	2698	2698	2698	2698	44	43	0
Hydrogen	kg/h	533	533	0	0	0	0	0	0	0	0	1885	1885	1885	1389	1389	1389	1389	1389	1389	1365	1351	14
Water	kg/h	0	0	0	0	0	0	0	0	0	0	12	12	12	1914	1914	1914	1914	1914	1914	12	12	0

1-Butanol	kg/h	0	0	0	0	0	0	0	0	0	0	16	16	16	9844	9844	9844	9844	9845	9845	16	16	0
Volume Flow	l/min	3650	2563	35641	15654	13058	5727	4341	1918	1330	775	9617	12050	13510	12721	12111	11622	11374	9063	7236	6874	6805	69

Table S3. (cont.).

Stream		**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**
Temperature	C	53	35	80	76	92	127	64	96	35	35	35	96	96	109	109	109	100	20	98	95	137	180
Pressure	bar	52	45	44	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	52	51	50
Molar Vapor Fraction		1	0	0	0	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Molar Liquid Fraction		0	1	1	1	0	1	0	1	1	1	0	1	1	1	1	1	1	1	1	1	1	1
Mole Flow	kmol/h	704	338	338	338	233	105	98	135	98	78	20	85	51	156	2	154	154	3	158	158	158	158
CO_2	kmol/h	30	5	5	5	5	0	5	0	5	0	5	0	0	0	0	0	0	0	0	0	0	0
CO	kmol/h	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	kmol/h	1	83	83	83	83	0	82	1	82	77	5	0	0	0	0	0	0	0	0	0	0	0
Hydrogen	kmol/h	670	12	12	12	11	1	11	0	11	0	11	0	0	1	0	1	1	0	1	1	1	1
Water	kmol/h	1	106	106	106	106	0	0	106	0	0	0	82	23	23	0	23	23	0	23	23	23	23
1-Butanol	kmol/h	0	133	133	133	29	104	0	29	0	0	0	2	27	131	1	129	129	3	133	133	133	133
Mass Flow	kg/h	2784	14650	14650	14650	6974	7676	2892	4082	2892	2494	398	1644	2439	10114	101	10013	10013	256	10269	10269	10269	10269
CO_2	kg/h	1339	241	241	241	241	0	241	0	241	20	221	0	0	0	0	0	0	0	0	0	0	0
CO	kg/h	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	kg/h	43	2654	2654	2654	2654	0	2629	25	2629	2474	155	11	14	14	0	14	14	0	14	14	14	14
Hydrogen	kg/h	1351	24	24	24	21	3	21	0	21	0	21	0	0	3	0	3	3	0	3	3	3	3

Water	kg/h	12	1902	1902	1902	1902	0	0	1902	0	0	0	1481	421	421	4	417	417	0	417	417	417	417
1-Butanol	kg/h	16	9828	9828	9828	2156	7673	0	2156	0	0	0	152	2004	9676	97	9580	9580	256	9835	9835	9835	9835
Volume Flow	l/min	6262	362	412	7488	83238	185	37742	83	7435	53	7382	30	52	3671	37	3634	226	5	231	261	278	306

1. Mass balances

Table S4. Component mass balance of the gas-phase CO_2 hydrogenation to methanol process.

In	**kg/h**					
Component	Stream					
	1	3	sum			
CO_2	0.0	3881.7	3881.7			
CO	0.0	0.0	0.0			
Methanol	0.0	0.0	0.0			
Hydrogen	533.2	0.0	533.2			
Water	0.0	0.0	0.0			
sum	533.2	3881.7	4414.9			
Out	kg/h					
Component	Stream					
	22	27	31	33	34	sum
CO_2	345.1	198.8	0.0	14.2	2.0	559.8
CO	77.7	4.8	0.0	0.0	0.0	82.5
Methanol	6.0	22.7	15.2	2274.8	0.5	2319.2
Hydrogen	84.7	4.0	0.0	0.0	0.0	88.6
Water	0.7	2.6	1355.5	1.0	0.0	1359.8
sum	514.2	232.4	1370.7	2289.9	2.6	4409.9

Table S5. Component mass balance of the liquid-phase CO_2 hydrogenation to methanol process in 1-butanol solvent.

In	**kg/h**					
Component	Stream					
	1	3	40			
CO_2	0.0	3881.7	0.0	3881.7		
CO	0.0	0.0	0.0	0.0		
Methanol	0.0	0.0	0.0	0.0		
Hydrogen	533.2	0.0	0.0	533.2		
Water	0.0	0.0	0.0	0.0		
1-butanol	0.0	0.0	255.7	255.7		
sum	533.2	3881.7	255.7	**4670.6**		
Out	kg/h					
Component	Stream					
	22	32	33	34	37	
CO_2	13.5	20.1	220.8	0.0	0.0	254.5
CO	0.2	0.0	0.4	0.0	0.0	0.7
Methanol	0.4	2474.2	155.2	11.0	0.1	2641.0
Hydrogen	13.7	0.0	21.2	0.0	0.0	34.9
Water	0.1	0.0	0.0	1480.6	4.2	1484.9
1-butanol	0.2	0.0	0.0	152.0	96.8	248.9
sum	28.1	2494.4	397.6	1643.5	101.1	**4664.8**

Table S6. Component mass balance of the liquid-phase CO_2 hydrogenation to methanol process in 2-butanol solvent.

In	**kg/h**			
Component	Stream			
	1	3	40	sum
CO_2	0.0	3881.7	0.0	3881.7
CO	0.0	0.0	0.0	0.0
Methanol	0.0	0.0	0.0	0.0
Hydrogen	533.2	0.0	0.0	533.2

Water	0.0	0.0	0.0	0.0		
2-butanol	0.0	0.0	296.5	296.5		
sum	533.2	3881.7	296.5	**4711.4**		
Out	kg/h					
Component	Stream					
	22	32	33	34	37	sum
CO_2	13.8	18.2	336.7	0.0	0.0	368.7
CO	0.2	0.0	0.4	0.0	0.0	0.6
Methanol	0.3	2311.3	254.4	2.3	0.1	2559.4
Hydrogen	16.4	0.0	34.0	0.0	0.1	50.6
Water	0.1	0.0	0.0	1429.4	11.5	1441.0
2-butanol	0.5	0.0	0.0	142.1	209.6	352.2
sum	31.5	2329.5	616.5	1573.8	221.2	**4772.4**

2. Thermal and electric duties of individual equipment

Table S7. Thermal duties (kW) in the gas-phase CO_2 hydrogenation to methanol process.

Equipment ID	Duty
COOLER1	-81.2
COOLER2	-96.3
COOLER3	-106.9
HX2	-1151.3
HX4	-760.1
DIST1 condenser	-764.3
Hot utility	
Cold utility	-2960.1
Integrated:	
HX1	3414.9
HX3	748.9
DIST1 reboiler	940.2
sum	5103.9

Table S8. Thermal duties (kW) in the liquid-phase CO_2 hydrogenation to methanol processes.

Equipment ID	2-butanol	1-butanol
COOLER1	-81.2	-81.2
COOLER2	-96.3	-96.3
COOLER3	-106.9	-106.9
HX2	389.5	376.9
HX5	-3595.1	-1775.1
HX6	-771.9	-826.3
HX7	-273.4	-176.3
HX8	1112.7	456.6
DIST1 reboiler	7282.2	5444.7
DIST1 condenser	-3642.2	-2678.3
DIST2 reboiler	1931.0	Integrated
DIST2 condenser	-6746.0	-3863.4
Hot utility	10715.4	6278.2
Cold utility	-15312.8	-9603.8
Integrated:		
HX1	827.8	760.1

HX3	1153.1	610.4
HX5	1115.4	411.5
DIST2 reboiler	2279.4	2265.0
sum	5375.7	4047.0

Table S9. Electric duties (kW) in the alternative CO_2 hydrogenation to methanol processes.

Equipment ID	Gas-phase	2-butanol	1-butanol
COMP1	93.2	93.2	93.2
COMP2	95.5	95.5	95.5
COMP3	93.3	93.3	93.3
COMP4	54.9	56.5	56.5
COMP5	132.0	137.4	137.4
COMP6	155.0	123.7	103.4
PUMP1		83.0	45.7
sum	624.0	682.6	625.1

3. Detailed capital and operating costs

Table S10. Installed equipment costs of the alternative CO_2 hydrogenation to methanol processes (M€).

Equipment type	Gas-phase	2-butanol	1-butanol
Compressors and pumps	7.3	7.3	7.2
Reactor	1.0	0.6	0.6
Separation*	1.4	4.0	2.8
Heat exchangers	0.8	1.1	1.0
Total	10.5	12.9	11.6

* Includes distillation and flash vessels.

Table S11. Operating and total methanol production costs of the alternative CO_2 hydrogenation to methanol processes (k€/t MeOH). Negative costs constitute revenues.

	Gas-phase	2-butanol	1-butanol
Hydrogen	702.4	646.5	654.7
Carbon dioxide	85.2	78.4	79.4
Total raw materials	787.7	724.9	734.1
Oxygen	-65.1	-59.9	-60.6
Waste water	0.2	0.2	0.2
Total byproducts and waste	-64.9	-59.7	-60.4
Electricity	13.2	16.6	12.8
Steam	-57.2	259.7	174.0
Cooling Water	43.2	89.2	54.9
Total utilities	-1.1	365.5	241.7
Catalyst	4.6	1.7	1.7
Solvent make-up		71.2	50.9
Total consumables	4.6	72.9	52.7
Variable costs, k€/t MeOH	726.3	1103.6	968.1
Labor and supervision	63.7	58.6	59.3
Maintenance	17.3	-9.6	18.3
Overheads, tax and insurance	68.9	69.2	67.7
Fixed costs, k€/t MeOH	149.9	147.4	145.3

Annual capital charge, k€/t MeOH	86.8	98.3	91.8
Total cost, k€/t MeOH	963.0	1349.4	1205.1

4. Calculations

Capacity of methanol synthesis

The capacity of the electrolysis unit is 30 MW. The amount of water consumed in electrolysis is calculated based on the heat of formation of water (258.8 kJ/mol) and the overall efficiency of the electrolysis unit, assumed 70% [S1]:

$$\dot{n}_{water} = 3600\ \frac{\mathrm{s}}{\mathrm{h}} * \frac{70\% * 30\ \mathrm{MW}}{258.8\,\frac{\mathrm{kJ}}{\mathrm{mol}}} = 264.5\ \mathrm{kmol/h}$$

One mole of hydrogen and 0.5 moles of oxygen are formed per mole of water consumed in electrolysis:

$$2\ \mathrm{H_2O} \rightarrow 2\ \mathrm{H_2} + \mathrm{O_2}$$

Thus, 264.5 kmol/h of hydrogen is available for methanol synthesis, and 132.3 kmol/h of oxygen is produced as by-product. In CO_2 hydrogenation to methanol, 3 moles of hydrogen are consumed per one mole of CO_2, and the amount of CO_2 input to the methanol synthesis process is thus 88.2 kmol/h. At full conversion to methanol, 88.2 kmol/h of methanol is formed. The amount of methanol output from the modelled methanol synthesis processes is compared to this theoretical value to obtain the overall methanol yield.

Cost of steam

Process heat is provided by medium-pressure (MP) steam at 20 bar (saturation temperature 212 °C) and low-pressure (LP) steam at 6 bar (159 °C). The cost of LP steam was assumed identical to the cost of MP steam, i.e. shaft work or condensate credits were not considered. The cost of boiler feed water was also omitted. Based on the enthalpies of steam at 212 °C (3025 kJ/kg) and boiler feed water at 100 °C (420 kJ/kg), the heat duty required to heat the boiler feed water to the saturation temperature of MP steam is

$$\Delta H = (3025 - 420)\frac{\mathrm{kJ}}{\mathrm{kg}} = 2605\ \frac{\mathrm{kJ}}{\mathrm{kg}}$$

Assuming 80% boiler efficiency and a fuel (natural gas) cost of 30 MWh [S2], the fuel cost is

$$\mathrm{C_{fuel}} = 8.33\ \cdot 10^{-6}\frac{€}{\mathrm{kJ}}\left(\frac{2605\ \frac{\mathrm{kJ}}{\mathrm{kg}}}{80\%}\right) = 0.027\ \frac{€}{\mathrm{kg}}$$

A correction factor of 1.3 was then employed to take non-fuel costs into account [S3], giving the total cost of 0.035 €/kg for MP steam. By the procedure above, a cost of 0.037 €/kg is obtained for HP steam (40 bar, saturation temperature 250 °C) required in the water adsorption unit. In the 1-pentanol process with water adsorption, the cost of MP and LP steam are is set at 0.035 €/kg regardless of the need to generate HP steam.

Cost of catalyst

In the gas-phase methanol synthesis unit, the catalyst is contained in 1000 tubes of 2 m in length and 0.05 m in diameter. Thus the total volume of the tubes is

$$V = \pi \cdot \left(\frac{0.05\ \mathrm{m}}{2}\right)^2 \cdot 2\ \mathrm{m} \cdot 1000 = 3.93\ \mathrm{m}$$

Catalyst density of 1775 kg/m³ [S4] and bed porosity of 0.5 are assumed. Thus the mass of catalyst in the tubes is

$$3.93\ \mathrm{m} \cdot 1775\ \frac{\mathrm{kg}}{\mathrm{m}^3} \cdot 0.5 = 3485\ \mathrm{kg}$$

Assuming a catalyst lifetime of 4 years, an average of 871 kg of catalyst is replaced per year. Assuming a catalyst price of 95.24 €/kg [S5], the cost per year is 83 983 €.

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