

Supplementary Information

Thermo-economic Analysis of integrated hydrogen, methanol and dimethyl ether production using water electrolyzed hydrogen

Table S1. Results of mass and energy balance for hydrogen production process by alkaline water electrolysis (AEL) corresponding to Figure 3 of the manuscript.

Stream	H ₂ O	KOH	TOHX1	TOPUMP	TOREAC	TOSEP	OXYGEN	L1	HYDROGEN	LIQ	REKOH
T (°C)	25	25	25	65	66	65	65	65	65	65	65
P (bar)	1	1	1	1	25	25	25	25	25	25	1
Mass Flows (kg/hr)											
Total	675	236	911	911	911	911	598	312	75	237	237
CH ₃ OH	0	0	0	0	0	0	0	0	0	0	0
H ₂ O	675	0	675	675	675	0.675	0	0.675	0	0.67	0.67
KOH	0	236	236	236	236	236	0	236	0	236	236
CO ₂	0	0	0	0	0	0	0	0	0	0	0
H ₂	0	0	0	0	0	75	0	75	75	0	0
O ₂	0	0	0	0	0	598	598	0	0	0	0
Energy Balance											
Heat duty (kJ/s) for HEAT1	33				Work (kJ/s) for P1				1		

Table S2. Results of mass and energy balance for hydrogen production process by proton exchange membrane (PEM) corresponding to Figure 4 of the manuscript.

Stream	H2O	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	H2OAN	H2OAT
T (°C)	25	25	80	80	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	141	90	90
P (bar)	1	1	1	25	25	25	25	25	25	25	25	25	20	25	25	25	20	20	20	35	20	25
Mass Flows (kg/hr)																						
Total	376	377	377	377	377	42	41	0.42	45	45	41	3	0.42	334	331	3.34	331	331	331	41	0.37	0.003
CH3OH	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2O	376	377	377	377	0.37	0	0	0	0	0	0	0	0	0	0.3	0	0.3	0.3	0	0	0.37	0.003
CO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2	0	0	0	0	42	0	0	0	42	42	41	3	0.42	0	0	0	0	0.42	0.42	41	0	0
O2	0	0	0	0	334	42	41	0.42	4	0	0	0	0	334	330	3.34	330	330	330	0	0	0
Energy Balance																						
Heat duty (kJ/s) for HEAT1					24		Work (kJ/s) for P1					0.38		Duty (kJ/s) for R1					1650			

Table S3. Results of mass balance for hydrogen production process solid oxide electrolyzer (SOE) corresponding to Figure 5 of the manuscript.

Stream 1 to 14														
Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14
T (°C)	25	25	66	101	115	113	111	800	800	800	800	800	118	800
P (bar)	1	2	1.9	1.8	1.7	1.6	1.5	1.3	1	1	1	1	1	1.0
Mass Flows (kg/hr)														
Total	110326	110326	110326	110326	110326	110326	110326	110326	111894	111894	15680	96213	96213	1568
CH ₃ OH	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H ₂ O	110326	110326	110326	110326	110326	110326	110326	110326	110547	2211	2211	0	0	221
CO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO ₂	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H ₂	0	0	0	0	0	0	0	0	1347	13470	13470	0	0	1347
O ₂	0	0	0	0	0	0	0	0	0	96213	0	96213	96213	0
Stream 15 to 27														
Stream	15	16	17	18	19	20	21	22	23	24	25	26	27	
T (°C)	800	116	25	25	178	71	38	197	106	38	198	120	38	
P (bar)	1.0	1.2	1.1	1.1	3.3	3.2	3.1	9.3	9.2	9.1	27.3	27.1	27	
Mass Flows (kg/hr)														

Total	14112	14112	1946	12166	12166	12166	12166	12166	12166	12166	12166	12166	12166
CH₃OH	0	0	0	0	0	0	0	0	0	0	0	0	0
H₂O	1989	1989	1946	43	43	43	43	43	43	43	43	43	43
CO	0	0	0	0	0	0	0	0	0	0	0	0	0
CO₂	0	0	0	0	0	0	0	0	0	0	0	0	0
H₂	12123	12123	0	12123	12123	12123	12123	12123	12123	12123	12123	12123	12123
O₂	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S4. Results of energy balance for hydrogen production process solid oxide electrolyzer (SOE) corresponding to Figure 5 of the manuscript.

Component	HX1	HX2	HX3	HX4	HX5	HX6	HX7	HX8	HX9	HX10	SOEC-1
Heat Duty (kJ/s)	5221	4479	3792	18790	34607	57365	-5844	-1588	-3285	-4006	414775
Component	CP1	CP2	CP3	CP4	P1						
Work (kJ/s)	7830	8184	8236	8077	3						

Table S5. Results of mass balance for methanol production process corresponding to Figure 6 of the manuscript.

Stream	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
T (°C)	192	28	60	38	158	38	126	38	136	167	67	212	285	285	94	94
P (bar)	78	2.0	3.0	2.7	8.8	8.7	26.3	26.0	78.0	78.0	78.0	75.7	75.1	75.1	74.8	73.6
Mass Flows (kg/hr)																
Total	12166	88736	88736	88736	88736	88736	88736	88736	88736	100902	411179	411179	411179	246707	246707	246707
CH ₃ OH	0	0	0	0	0	0	0	0	0	0	5477	5477	67641	40584	40584	40584
H ₂ O	44	735	735	735	735	735	735	735	735	779	1308	1308	36404	21843	21843	21843
CO	0	0	0	0	0	0	0	0	0	0	45144	45144	45371	27223	27223	27223
CO ₂	0	88000	88000	88000	88000	88000	88000	88000	88000	88000	272574	272574	186837	112102	112102	112102
H ₂	12123	0	0	0	0	0	0	0	0	12123	8,675	86675	74926	44955	44955	44955
O ₂	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stream	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59
T (°C)	285	166	76	87	35	35	35	35	35	42	34	28	29	29	688	80
P (bar)	75.1	74.6	73.6	73.6	73.4	73.4	73.4	73.4	73.4	78.0	10.0	1.2	1.2	1.2	78	1.1
Mass Flows (kg/hr)																
Total	164471	16471	164471	411178	411178	104408	306770	1534	305236	305236	104408	104408	102219	2188	2188	102219
CH ₃ OH	27056	27056	27056	67640	67640	63371	4270	21	4248	4248	63371	63371	62949	421	421	62949
H ₂ O	14562	14562	14562	36404	36404	35919	486	2	483	483	35919	35919	35872	45	45	35872
CO	18148	18148	18148	45371	45371	131	45240	226	45014	45014	131	131	12	118	118	12
CO ₂	74735	74735	74735	186836	186836	4822	182015	910	181105	181105	4822	4822	3384	1437	1437	3384
H ₂	29970	29970	29970	74926	74926	167	74759	374	74386	74386	167	167	0	166	166	0
O ₂	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stream	60	61	62	63	64	65	66	67	Streams for ORC							
T (°C)	102	63	78	40	40	40	512	46	Stream	A	B	C	D	E		
P (bar)	T (°C)	1	1.2	1	1	1	78	78	T	97	57	33	34	102		
Mass Flows (kg/hr)									P (bar)	12	2	2	12	1		
Total	35819	66400	66400	66400	63547	2852	2852	310276	Total	4500	4500	4500	4500	35747		
CH ₃ OH	0	62949	62949	62949	62141	808	808	5477	R-245fa	4500	4500	4500	4500	0		
H ₂ O	35819	53	53	53	53	0	0	529	H ₂ O	0	0	0	0	35747		
CO	0	12	12	12	0	11	11	45144								
CO ₂	0	3384	3384	3384	1352	2032	2032	184574								
H ₂	0	0	0	0	0	0	0	74552								
O ₂	0	0	0	0	0	0	0	0								

Table S6. Results of energy balance for methanol production process corresponding to Figure 6 of the manuscript.

Component	REB	DTC	H1	HX11	HX12	HX13	HX14	HX15	HX16	HX18	COND
Heating/cooling duty (kJ/s)	-21129	-24146	290	-468	-3345	-2643	68791	28905	-35834	-20844	261
Component	P1	TUR	CP5	CP6	CP7	CP8	CP9	CP10	CP11	CP12	
Work (kJ/s)	1	-27	902	2998	2551	2390	448	1043	2942	530	

Table S7. Results of mass and energy balance for DME production process corresponding to Figure 7 of the manuscript.

Stream	FEED	1	2	3	4	5	6	7	8	Waste	Recycle	DME
Temp. (°C)	40	40	64	153	350	150	90	167	138	180	138	61
Press. (bar)	1	15	15	15	14	14	15	15	10	10	15	15
Mass Flows (kg/hr)												
Total	62120	62120	78321	78320	78321	78321	78321	33666	16201	17464	16201	44653
CH ₃ OH	62120	62120	77647	77647	15528	15528	15528	15528	15528	0.97	15528	0.17
H ₂ O	0	0	673	673	18137	18137	18137	18137	673	17463	673	0
CO	0	0	0	0	0	0	0	0	0	0	0	0
CO ₂	0	0	0	0	0	0	0	0	0	0	0	0
H ₂	0	0	0	0	0	0	0	0	0	0	0	0
DME	0	0	0.003	0.003	44653	44653	44653	0.003	0.003	0	0.003	44653
Energy Balance												
Component	HE1		R1		CHILL1		DTC1		DTC2			
Heating/Cooling duty (kJ/s)	14923		14864		-15609		-63431		-10879			
Component	P1		P2									
Work (kJ/s)	34		6									