

Supplementary Materials

Multi-Scale Analysis of Integrated C₁ (CH₄ & CO₂) Utilization Catalytic Processes: Impacts of Catalysts Characteristics up to Industrial-Scale Process Flowsheeting

Part II: Techno-Economic Analysis of Integrated C₁ Utilization Process Scenarios

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Table S-1. Set of operating conditions and simulated results predicting the compositions of the main streams in the integrated process scenario 5 (Int-Sec-5).

Scenario 5	OCM Reactor		EDH Reactor		Cooling Section		First CO ₂ Removal		CO ₂ hydrogenation			Demethanizer		
	Inlet	Outlet	Inlet	Outlet	Inlet	Outlet	Inlet	Outlet	Inlet	To Reformer	Methanol	Inlet	Top	Bottom
Temperature [°C]	650	600	835	650	375	30	30	0	249	18	40	5	-109	2
Pressure [bar]	9.9	9.8	10.0	10.0	9.8	9.5	9.5	9.7	10.0	6.0	1.4	33.6	33.4	33.4
Mole Flow [Mmol/hr]	98.5	104.2	4.6	5.3	109.0	84.8	84.8	48.0	58.6	29.4	6.2	30.4	11.4	0.7
Mole Frac														
Oxygen	0.232	0.015	0.110		0.015									
Methane	0.464	0.248		0.017	0.245	0.305	0.305	0.539	264 PPM	221 PPM	117 PPB	0.539	0.661	556 PPM
Ethane		0.014	0.525	0.195	0.014	0.029	0.029	0.052	24 PPM	20 PPM	49 PPB	0.052	6 PPM	0.280
Propane				0.017	0.012	0.002	0.002	0.003	1 PPM	924 PPB	2 PPB	0.003	8 PPB	0.016
Ethylene		0.043	0.005	0.243	0.041	0.068	0.068	0.120	163 PPM	136 PPM	310 PPB	0.120	121 PPM	0.644
Propylene		0.005	0.003	0.005	0.005	0.006	0.006	0.011	25 PPM	21 PPM	81 PPB	0.011	46 PPB	0.060
Carbon monoxide		0.040		0.001	0.038	0.049	0.049	0.087	30 PPM	0.109	6 PPM	0.087	0.106	13 PPB
Carbon dioxide	0.305	0.349		0.001	0.333	0.429	0.429	30 PPM	0.247	0.165	0.004	30 PPM	10 PPB	163 PPM
Hydrogen		0.086		0.018	0.106	0.107	0.107	0.189	0.742	0.714	30 PPM	0.189	0.232	trace
Water		0.200	0.357	0.501	0.190	0.004	0.004		0.010	0.003	0.002			
Methanol										0.009	0.995			

Scenario 5	Ethylene Splitter			Ethane Splitter			Refomer		H2 Paladium Membrane			Second CO2	
	Inlet	Ethylene	Bottom	Inlet	Ethane	C3+	Inlet	Outlet	Inlet	H2	Syngas	Inlet	Syngas
Temperature [°C]	-19	-31	-1	-3	-20	31	850	850	250	250	250	250	40
Pressure [bar]	20.0	18.9	18.9	18.0	14.0	14.0	10.2	10.1	10.1	10.0	10.1	10.1	9.5
Mole Flow [Mmol/hr]	8.9	5.7	3.2	3.2	2.5	0.7	111.5	133.5	133.5	43.5	119.5	119.5	97.9
Mole Frac													
Oxygen													
Methane	556 PPM	862 PPM	trace	trace			0.232	845 PPM	845 PPM		999 PPM	999 PPM	0.001
Ethane	0.280	0.004	0.780	0.780	0.984	0.039	7 PPM	2 PPM	2 PPM		7 PPM	7 PPM	8 PPM
Propane	0.016	trace	0.044	0.044	631 PPM	0.202	247 PPB	2 PPB	2 PPB		230 PPB	230 PPB	281 PPB
Ethylene	0.644	0.995	0.007	0.007	0.009	20 PPM	78 PPM	35 PPM	35 PPM		73 PPM	73 PPM	89 PPM
Propylene	0.060	trace	0.169	0.169	0.006	0.759	5 PPM	14 PPB	14 PPB		5 PPM	5 PPM	6 PPM
Carbon monoxide	13 PPB	20 PPB	trace	trace			0.066	0.191	0.191		0.240	0.240	0.294
Carbon dioxide	163 PPM	241 PPM	23 PPM	23 PPM	29 PPM	106 PPB	0.043	0.033	0.033		0.079	0.079	188 PPM
Hydrogen	trace	trace	trace	trace			0.270	0.679	0.679	1	0.570	0.570	0.697
Water							0.386	0.097	0.097		0.109	0.109	0.007
Methanol							0.002						