

Optimization of Methyl Chloride Production from Methanol and Hydrogen Chloride by Enhancing Purity and Reducing Total Energy Demand

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Table S1. Mass and energy balance of the basic process of methyl chloride production

		14	HCl	Methanol	1	2	3	5	6	7	11
Vapour Fraction		0.0000	0.6020	0.6020	0.6020	1.0000	1.0000	0.5897	1.0000	0.0000	0.0000
Temperature	C	130.8	40.00	40.00	40.00	105.0	105.0	40.00	29.96	30.36	30.36
Pressure	atm	3.069	2.961	2.961	2.961	2.961	2.961	2.961	2.961	2.961	2.961
Molar Flow	kgmole/h	2.467e+004	331.1	471.4	802.4	802.4	798.5	798.5	448.5	2.468e+004	2.469e+004
Mass Flow	kg/h	4.457e+005	1.142e+004	1.626e+004	2.768e+004	2.768e+004	2.797e+004	2.797e+004	2.081e+004	4.462e+005	4.463e+005
Liquid Volume Flow	m ³ /h	447.2	13.63	19.41	33.04	33.04	30.45	30.45	22.97	447.8	447.9
Heat Flow	kJ/h	-6.853e+009	-5.154e+007	-7.338e+007	-1.249e+008	-1.108e+008	-1.191e+008	-1.354e+008	-4.047e+007	-7.048e+009	-7.050e+009
	H ₂ O	8	9	10	12	18	4	13	15	16	
Vapour Fraction		0.0000	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Temperature	C	30.00	40.00	34.78	34.85	30.36	-37.65	105.0	-37.69	40.00	40.00
Pressure	atm	2.961	2.961	2.961	2.961	2.961	3.069	2.961	3.069	3.069	3.069
Molar Flow	kgmole/h	6.828	448.5	450.6	4.725	2.469e+004	13.41	17.34	13.41	2.467e+004	6.810
Mass Flow	kg/h	123.0	2.081e+004	2.085e+004	85.25	4.463e+005	611.2	323.7	610.9	4.457e+005	123.0
Liquid Volume Flow	m ³ /h	0.1232	22.97	23.01	8.545e-002	447.9	0.6776	0.3307	0.6773	447.2	0.1234
Heat Flow	kJ/h	-1.952e+006	-4.029e+007	-4.088e+007	-1.348e+006	-7.050e+009	-1.480e+006	-4.821e+006	-1.480e+006	-7.030e+009	-1.940e+006
	17	19	20	21	22	23	24	25	26	27	
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Temperature	C	40.00	40.00	30.00	30.00	40.05	39.26	88.31	88.34	88.34	30.00
Pressure	atm	3.069	2.961	2.961	2.961	0.6579	0.6579	0.6579	2.961	2.961	2.961
Molar Flow	kgmole/h	2.457e+004	6.810	6.810	6.805	2.467e+004	130.0	2.454e+004	2.454e+004	2.454e+004	2.433e+004
Mass Flow	kg/h	4.455e+005	123.0	123.0	123.0	4.455e+005	2822	4.427e+005	4.427e+005	4.427e+005	4.389e+005
Liquid Volume Flow	m ³ /h	447.1	0.1234	0.1234	0.1235	447.1	3.067	444.0	444.0	444.0	440.2
Heat Flow	kJ/h	-7.028e+009	-1.940e+006	-1.945e+006	-1.944e+006	-7.028e+009	-3.505e+007	-6.870e+009	-6.870e+009	-6.979e+009	-6.919e+009

Compositions										
	14	HCl	Methanol	1	2	3	5	6	7	11
Comp Mole Frac (Methanol)	0.0031	0.4450	0.4450	0.4450	0.4450	0.0348	0.0348	0.0000	0.0031	0.0031
Comp Mole Frac (HCl)	0.0000	0.5550	0.5550	0.5550	0.5550	0.1522	0.1522	0.2585	0.0002	0.0002
Comp Mole Frac (Refrig-40)	0.0001	0.0000	0.0000	0.0000	0.0000	0.4223	0.4223	0.7269	0.0005	0.0005
Comp Mole Frac (H ₂ O)	0.9968	0.0000	0.0000	0.0000	0.0000	0.3907	0.3907	0.0145	0.9962	0.9962
	H ₂ O	8	9	10	12	18	4	13	15	16
Comp Mole Frac (Methanol)	0.0000	0.0000	0.0001	0.0005	0.0031	0.0000	0.0444	0.0000	0.0031	0.0031
Comp Mole Frac (HCl)	0.0000	0.2585	0.2574	0.0002	0.0002	0.3512	0.0002	0.3519	0.0000	0.0000
Comp Mole Frac (Refrig-40)	0.0000	0.7269	0.7236	0.0005	0.0005	0.6488	0.0007	0.6481	0.0001	0.0001
Comp Mole Frac (H ₂ O)	1.0000	0.0145	0.0190	0.9968	0.9962	0.0000	0.9547	0.0000	0.9968	0.9968
	17	19	20	21	22	23	24	25	26	27
Comp Mole Frac (Methanol)	0.0031	0.0031	0.0031	0.0040	0.0031	0.2103	0.0020	0.0020	0.0020	0.0020
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Refrig-40)	0.0001	0.0001	0.0001	0.0001	0.0001	0.0190	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H ₂ O)	0.9968	0.9968	0.9968	0.9959	0.9968	0.7641	0.9980	0.9980	0.9980	0.9980

Energy Streams								
		Q1	Q2	Q3	Qc	Qr	Q5	Q6
Heat flow	kJ/h	1.415e+07	-1.167e+07	1.634e+07	1.057e+07	1.964e+07	0.0000	1.77e+08
		Q7	Qc1	Qr1	Q8	Q9	Q4	
Heat flow	kJ/h	5304	2,495e+07	1,1480e+08	1,440e+05	1,087e+08	1,796e+05	

Table S2. Mass and energy balance of the modified process for methyl chloride production

Material Streams										
		HCl	Methanol	1	2	3	4	5	6	
Vapour Fraction		0.6020	0.6020	0.6020	1.0000	1.0000	1.0000	0.6052	1.0000	
Temperature	C	40.00	40.00	40.00	105.0	105.0	105.0	40.00	40.00	
Pressure	atm	2.961	2.961	2.961	2.961	2.961	2.961	2.961	2.961	
Molar Flow	kgmole/h	331.1	471.4	802.4	802.4	757.9	3.676e+004	757.9	458.7	
Mass Flow	kg/h	1.142e+004	1.626e+004	2.768e+004	2.768e+004	2.700e+004	6.634e+005	2.700e+004	2.160e+004	
Liquid Volume Flow	m ³ /h	13.63	19.41	33.04	33.04	29.18	665.1	29.18	23.76	
Heat Flow	kJ/h	-5.154e+007	-7.338e+007	-1.249e+008	-1.108e+008	-1.121e+008	-1.029e+010	-1.270e+008	-4.176e+007	
		7	13	H ₂ O	8	9	10	11	12	
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0001	0.0001	
Temperature	C	40.00	40.00	30.00	40.00	39.89	40.00	105.0	105.0	
Pressure	atm	2.961	2.961	2.961	2.961	2.961	2.961	2.961	2.961	
Molar Flow	kgmole/h	299.2	300.1	6.828	3.676e+004	456.8	3.677e+004	3.677e+004	3.642e+004	
Mass Flow	kg/h	5397	5415	123.0	6.634e+005	2.154e+004	6.636e+005	6.636e+005	6.573e+005	
Liquid Volume Flow	m ³ /h	5.409	5.429	0.1232	665.1	23.69	665.3	665.3	659.1	
Heat Flow	kJ/h	-8.525e+007	-8.525e+007	-1.952e+006	-1.047e+010	-4.157e+007	-1.048e+010	-1.029e+010	-1.019e+010	

Compositions								
	HCl	Methanol	1	2	3	4	5	6
Comp Mole Frac (Methanol)	0.4450	0.4450	0.4450	0.4450	0.0006	0.0008	0.0006	0.0000
Comp Mole Frac (HCl)	0.5550	0.5550	0.550	0.5550	0.1112	0.0001	0.1112	0.1827
Comp Mole Frac (H2O)	0.0000	0..0000	0.0000	0.0000	0.4093	0.9985	0.4093	0.0253
Comp Mole Frac (Refrig-40)	0.0000	0..0000	0..0000	0.0000	0.4789	0.0005	0.4789	0.7920
	7	13	H2O	8	9	10	11	12
Comp Mole Frac (Methanol)	0.0001	0.0008	0.0000	0.0008	0.0000	0.0008	0.0008	0.0010
Comp Mole Frac (HCl)	0.0002	0.0002	0.0000	0.0001	0.1797	0.0002	0.0002	0.0002
Comp Mole Frac (H2O)	0.9992	0.9985	1.0000	0.9985	0.0252	0.9985	0.9985	0.9983
Comp Mole Frac (Refrig-40)	0.0005	0.0005	0.0000	0.0005	0.7951	0.0005	0.0005	0.0005

Energy Streams							
		Q1	Q2	Q3	Q4	Q5	Q6
Heat flow	kJ/h	1.415e+07	-1.288e+07	1.495e+07	-1.281e+04	1.874e+08	1.875e+08