

Energy Optimization of Dimethyl Ether (DME) Production Process from Methanol Dehydration

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Table S1. Mass and Energy Balances

Data	Unit	Feed	1	2	3	4	5	6	7	8	9	DME	10	Methanol Recycle	Wastewater
Vapour Fraction		0.00	0.00	0.00	0.80	1.00	1.00	1.00	0.00	0.00	0.16	0.00	0.00	0.00	0.00
Temperature	C	30.00	32.84	33.37	141.61	191.81	308.51	227.84	80.89	81.04	100.00	3.92	136.04	132.00	135.11
Pressure	atm	1.00	1.00	10.86	10.86	32.92	32.43	32.23	32.23	10.00	10.00	3.00	3.20	3.00	3.10
Molar Flow	kgmole/h	83.10	86.71	86.71	86.71	86.71	86.71	86.71	86.71	86.71	86.71	41.47	45.24	3.61	41.60
Mass Flow	kg/h	2660.58	2726.32	2726.32	2726.32	2726.32	2726.34	2726.34	2726.34	2726.34	2726.34	1910.61	815.73	65.74	749.43
Master Comp Mass Flow (diM-Ether)	kg/h	0.00	0.20	0.20	0.20	0.20	1910.81	1910.81	1910.81	1910.81	1910.81	1910.61	0.21	0.20	0.00
Master Comp Mass Flow (H ₂ O)	kg/h	2.70	67.03	67.03	67.03	67.03	814.17	814.17	814.17	814.17	814.17	0.00	814.17	64.33	749.30
Master Comp Mass Flow (Methanol)	kg/h	2657.88	2659.08	2659.08	2659.08	2659.08	1.36	1.36	1.36	1.36	1.36	0.00	1.36	1.21	0.13
Heat Flow	kJ/h	-19855698	-20853419	-20848062	-17734585	-17238360	-17238030	-17734255	-20847732	-20847732	-20449621	-8536543	-12505066	-997721	-11503050
Phase Mass Flow (Liquid Phase)	kg/h	2660.58	2726.32	2726.32	539.99	0.00	0.00	0.00	0.00	0.00	0.00	1910.61	0.00	0.00	0.00
Phase Mass Flow (Vapour Phase)	kg/h	0.00	0.00	0.00	2186.33	2726.32	2726.34	2726.34	0.00	0.00	602.59	0.00	0.00	0.00	0.00
Phase Molecular Weight (Liquid Phase)		32.02	31.44	31.44	31.14	31.14	0.00	0.00	0.00	0.00	0.00	46.07	0.00	0.00	0.00
Phase Molecular Weight (Vapour Phase)		0.00	31.93	0.00	31.52	31.44	31.44	31.44	0.00	0.00	44.21	0.00	0.00	0.00	0.00
Phase Mass Density (Liquid Phase)	kg/m ³	780.97	782.12	782.15	653.64	568.79	0.00	0.00	0.00	0.00	0.00	633.14	0.00	0.00	0.00
Phase Mass Density (Vapour Phase)	kg/m ³	0.00	1.30	0.00	11.49	38.57	23.05	28.18	0.00	0.00	15.93	0.00	0.00	0.00	0.00
Phase Mass Density (Liquid Phase) - 2	kg/m ³	780.97	782.12	782.15	653.64	568.79	0.00	0.00	0.00	0.00	0.00	633.14	0.00	0.00	0.00
Phase Mass Density (Vapour Phase) - 2	kg/m ³	0.00	1.30	0.00	11.49	38.57	23.05	28.18	0.00	0.00	15.93	0.00	0.00	0.00	0.00
Phase Actual Volume Flow (Liquid Phase)	m ³ /h	3.41	3.49	3.49	0.83	0.00	0.00	0.00	0.00	0.00	0.00	3.02	0.00	0.00	0.00
Phase Actual Volume Flow (Vapour Phase)	m ³ /h	0.00	0.00	0.00	190.30	70.69	118.28	96.73	0.00	0.00	37.82	0.00	0.00	0.00	0.00
Phase Z Factor (Liquid Phase)		0.00	0.00	0.02	0.02	0.05	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
Phase Z Factor (Vapour Phase)		0.00	0.97	0.00	0.88	0.70	0.93	0.87	0.00	0.00	0.91	0.00	0.00	0.00	0.00

Data	Unit	Feed	1	2	3	4	5	6	7	8	9	DME	10	Methanol Recycle	Wastewater
Phase Cp/Cv (Liquid Phase)		1.37	1.35	1.35	1.38	1.44	0.00	0.00	0.00	0.00	0.00	1.64	0.00	0.00	0.00
Phase Cp/Cv (Vapour Phase)		0.00	1.25	0.00	1.32	1.75	1.20	1.26	0.00	0.00	1.18	0.00	0.00	0.00	0.00
Phase Viscosity (Liquid Phase)	cP	0.51	0.50	0.49	0.15	0.08	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00
Phase Viscosity (Vapour Phase)	cP	0.00	0.01	0.00	0.01	0.01	0.02	0.02	0.00	0.00	0.01	0.00	0.00	0.00	0.00
Phase Mass Heat Capacity (Liquid Phase)	kJ/kg-C	3.62	3.64	3.64	4.37	5.47	0.00	0.00	0.00	0.00	0.00	2.31	0.00	0.00	0.00
Phase Mass Heat Capacity (Vapour Phase)	kJ/kg-C	0.00	1.42	0.00	1.89	2.82	2.31	2.23	0.00	0.00	1.76	0.00	0.00	0.00	0.00
Phase Thermal Conductivity (Liquid Phase)	W/m-K	0.18	0.19	0.19	0.15	0.11	0.00	0.00	0.00	0.00	0.00	0.15	0.00	0.00	0.00
Phase Thermal Conductivity (Vapour Phase)	W/m-K	0.00	0.01	0.00	0.02	0.03	0.05	0.04	0.00	0.00	0.02	0.00	0.00	0.00	0.00