

Enhancing the Yield and Mass Production of Vinyl Chloride Production from Ethylene and Chloride through EDC Vapor Recovery in Direct Chlorination Process

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Table SI. Supporting information data (SI)

Stream Number	Unit	Ethylene	Cl2	S1	S5	S20	S6	S7	S8	S9	S10	S12	S11	S13	S14	S15	S16 (Vinyl Chloride)	S 17	S18	S 19	S2	S3	S4
Total Phase Properties																							
Temperature	C	25	25	65	65	65	34.6081019	34.6081	34.60810188	35.9998409	242	500	500	6	-21.8654	74.53045	65.99569	154.216	72.24536	65	10	10	10
Pressure	atm	1.5	1.5	1.5	1.5	1.5	1	1	1	26	26	26	26	12	11	11.5	11	11.25	1.603	1.5	1	1	1
Molar Flow	kgmole/h	90	90	59.93018	34.56982	10.07732	98.3270728	0.781015	97.54605756	97.5460576	97.5460576	181.6767	0	181.6767	104.5064	77.17025	67.01576	10.15449	10.15449	10.15449	59.93018	6.250246	53.67994
Mass Flow	kg/h	2524.842	6381.513	5494.594	3411.786	997.2494	9598.64047	54.37719	9544.263281	9544.26328	9544.26328	9543.672	0	9543.672	4347.288	5196.383	4191.497	1004.886	1004.886	1004.886	5494.594	304.9896	5189.605
Liquid Volume Flow	m3/h	6.588389	4.087258	4.805042	2.88361	0.843297	8.10582948	0.055366	8.050463351	8.05046335	8.05046335	10.25049	0	10.25049	4.852317	5.398169	4.548414	0.849755	0.849755	0.849755	4.805042	0.426119	4.378922
Heat Flow	kJ/h	4703353	-10630.8	6260781	5345560	1569998	15103550.2	-31082.2	15072468.01	15044580.5	10635809.1	1430533	0	9241180	8970792	-231675	1282486	1456637	1456637	1582021	8113308	74685.21	8187993
Vapor Phase Properties																							
Mass Flow	kg/h																						
Molecular Weight		28.0538	70.9057	91.68326	91.68326	<empty>	69.6237184	69.62372	69.62371842	<empty>	97.8436599	52.53108	52.53108	39.76103	<empty>	63.60115	<empty>	<empty>	98.95979	<empty>	48.79642	48.79642	48.79642
Mass Density	kg/m3	1.737163	4.429543	5.134121	5.134121	<empty>	2.80555913	2.805559	2.805559129	<empty>	77.9337228	21.75977	21.75977	23.41989	<empty>	31.02618	<empty>	<empty>	5.836044	<empty>	2.127119	2.127119	2.127119
Actual Gas Flow	ACT_m3/h	1453.429	1440.671	1070.211	0	<empty>	19.3819425	19.38194	0	<empty>	122.46641	438.5924	0	33.88979	<empty>	0.000881	<empty>	<empty>	69.42039	<empty>	143.3815	143.3815	0
Z Factor		0.990142	0.981451	0.965374	0.965374	<empty>	0.98269366	0.982694	0.982693663	<empty>	0.7722124	0.989376	0.989376	0.889419	<empty>	0.826312	<empty>	<empty>	0.959063	<empty>	0.987346	0.987346	0.987346
Cp/Cv		1.24199	1.342414	1.136603	1.136603	<empty>	1.18224339	1.182243	1.182243393	<empty>	1.23774522	1.163385	1.163385	1.510455	<empty>	1.301867	<empty>	<empty>	1.126349	<empty>	1.23435	1.23435	1.23435
Viscosity	cP	0.010194	0.013728	0.01051	0.01051	<empty>	0.01082499	0.010825	0.010824992	<empty>	0.01788148	0.029831	0.029831	0.01266	<empty>	0.011728	<empty>	<empty>	0.010227	<empty>	0.010276	0.010276	0.010276
Mass Heat Capacity	kJ/kg-C	1.578443	0.487442	0.848186	0.848186	<empty>	0.82043094	0.820431	0.820430938	<empty>	1.22262659	1.259504	1.259504	0.921383	<empty>	1.073028	<empty>	<empty>	0.860668	<empty>	0.936283	0.936283	0.936283
Thermal Conductivity	W/m-K	0.021461	0.009208	0.011592	0.011592	<empty>	0.01248968	0.01249	0.01248968	<empty>	0.02266583	0.042458	0.042458	0.016094	<empty>	0.01518	<empty>	<empty>	0.011245	<empty>	0.014496	0.014496	0.014496
Liquid Phase Properties																							
Mass Flow	kg/h	<empty>	<empty>	0	3411.786	997.2494	9544.26328	0	9544.263281	9544.26328	<empty>	0	0	8749.976	4347.288	5196.356	4191.497	1004.886	599.7459	1004.886	5189.605	0	5189.605
Molecular Weight		<empty>	<empty>	98.69263	98.69263	98.9598	97.8436599	97.84366	97.8436599	97.8436599	<empty>	52.46686	52.46686	54.10738	41.59829	67.33664	62.54495	98.9598	98.9598	98.9598	96.67681	96.67681	96.67681
Mass Density	kg/m3	<empty>	<empty>	1104.951	1104.951	1104.633	1155.92001	1155.92	1155.920009	1157.29587	<empty>	21.73213	21.73213	981.5245	1031.381	846.9966	816.7398	936.3539	1092.512	1104.633	1194.54	1194.54	1194.54
Actual Volume Flow	m3/h	<empty>	<empty>	0	3.087727	0.902788	8.25685446	0	8.256854458	8.24703823	<empty>	0	0	8.91468	4.215019	6.135038	5.131986	1.073191	0.54896	0.909702	4.344437	0	4.344437
Viscosity	cP	<empty>	<empty>	0.315484	0.315484	0.316858	0.41731831	0.417318	0.417318314	0.41227201	<empty>	0.007225	0.007225	0.199089	0.18641	0.134303	0.123818	0.149058	0.296624	0.316858	0.529586	0.529586	0.529586
Mass Heat Capacity	kJ/kg-C	<empty>	<empty>	1.261899	1.261899	1.262482	1.18851665	1.188517	1.188516647	1.18581699	<empty>	1.258512	1.258512	1.491283	1.718328	1.625882	1.681682	1.575737	1.280827	1.262482	1.135576	1.135576	1.135576
Surface Tension	dyne/cm	<empty>	<empty>	20.81421	20.81421	20.91103	24.8519916	24.85199	24.85199159	24.6493416	<empty>	0	<empty>	13.76762	12.26521	9.628317	9.247369	9.228849	19.89861	20.91103	28.05222	28.05222	28.05222

	Unit	Ethylene	Cl2	S1	S5	S20	S6	S7	S8	S9	S10	S12	S11	S13	S14	S15	S16 (Vinyl Chloride)	S 17	S18	S 19	S2	S3	S4
Composition																							
Comp Mole Frac (Ethylene)		1	0	0.074446	0.001111	1.00309E-30	0.006760132	0.315668116	0.00428682	0.00428682	0.00428682	0.000115	0.000115	0.000115	0.000200065	6.60397E-13	7.60463E-13	9.93171E-31	9.93171E-31	9.93171E-31	0.074446	0.613623	0.011667
Comp Mole Frac (Cl2)		0	1	0.071214	0.006714	2.02833E-13	0.03068922	0.24785386	0.028950463	0.028950463	0.028950463	0.013358	0.013352	0.013358	0.019965186	0.004409203	0.005077303	8.25082E-14	8.25082E-14	8.25082E-14	0.071214	0.237178	0.05189
Comp Mole Frac (11-ClC2)		0	0	0.854339	0.992174	0.9999999	0.962550637	0.436477974	0.966762707	0.966762707	0.966762707	0.055997	0.055576	0.055997	8.57509E-12	0.131829162	0.000280529	0.9999999	0.9999999	0.9999999	0.854339	0.149199	0.936443
Comp Mole Frac (VinylCl)		0	0	0	0	1.00173E-07	1.02665E-08	5.09956E-08	9.9404E-09	9.9404E-09	9.9404E-09	0.465265	0.463816	0.465265	0.171005458	0.863761535	0.994642053	9.98268E-08	9.98268E-08	9.98268E-08	0	0	0
Comp Mole Frac (HCl)		0	0	0	0	2.60627E-28	2.6711E-29	8.37936E-28	2.02159E-29	2.02159E-29	2.02159E-29	0.465265	0.467141	0.465265	0.808829291	1.0009E-07	1.15256E-07	2.54481E-28	2.54481E-28	2.54481E-28	0	0	0

	Unit	Q Reactor	Q P-100	Q HE-100	Q CRV-101	Q CO-101	Q Reb. T-100	Q Con. T-100	Q Con. T-101	Q Reb. T-101	Q CO-102	Q CO-100
Energy Stream												
Heat Flow	<i>kJ/h</i>	-16299063,4	27887,52	4408771	9205277	7810647	2373570	2335058	1573528	1631051	125383,8	1852526