

Enhancing Vinyl Chloride Product Yield by Optimizing Operating Conditions In Plug Flow Reactor With Al₂O₃ Catalyst

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Table S1. Mass and energy balance before process modification

Name	CL2	Ethylene	EDC Vapor	EDC liq 1	Mix
Vapour Fraction	1.0000	1.0000	1.0000	0.0000	0.0000
Temperature (C)	25.00 *	25.00 *	65.00 *	65.00	65.00
Pressure (atm)	1.500 *	1.500 *	1.500 *	1.500	1.500
Molar Flow (kgmole/h)	100.0 *	100.0 *	63.27	41.73	46.24
Mass Flow (kg/h)	7091	2805	5787	4109	4554
Liquid Volume Flow (m ³ /h)	4.541	7.320	5.017	3.482	3.859
Heat Flow (kJ/h)	-1.181e+004	5.226e+006	-7.117e+006	-6.419e+006	-7.120e+006
Name	Rich EDC	Heat Out	Vc vapor	L2	Vc Vapor 2
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	0.1203
Temperature (C)	66.55	242.0 *	500.0	500.0 *	6.000 *
Pressure (atm)	26.00 *	26.00 *	26.00	26.00	12.00 *
Molar Flow (kgmole/h)	46.24	46.24	87.37	0.0000	87.37
Mass Flow (kg/h)	4554	4554	4554	0.0000	4554
Liquid Volume Flow (m ³ /h)	3.859	3.859	4.936	0.0000	4.936
Heat Flow (kJ/h)	-7.106e+006	-5.163e+006	-6.599e+005	-0.0000	-4.404e+006
Name	HCl	VClq	Vinyl Chloride	EDCa	EDC recycle
Vapour Fraction	0.0000	0.0000	0.0000	0.0000	0.0000
Temperature (C)	-28.28	74.54	65.83	157.5	65.00 *
Pressure (atm)	11.05	12.00	11.05	12.00	1.500 *
Molar Flow (kgmole/h)	41.65	45.72	41.17	4.544	4.504 *
Mass Flow (kg/h)	1533	3021	2572	449.5	445.5
Liquid Volume Flow (m ³ /h)	1.759	3.177	2.797	0.3802	0.3768
Heat Flow (kJ/h)	-4.457e+006	1.129e+005	7.788e+005	-6.487e+005	-7.008e+005
Name	EDC cool				
Vapour Fraction	0.0000				
Temperature (C)	65.00 *				
Pressure (atm)	1.500 *				
Molar Flow (kgmole/h)	4.544				
Mass Flow (kg/h)	449.5				
Liquid Volume Flow (m ³ /h)	0.3802				
Heat Flow (kJ/h)	-7.071e+005				

Name	Unit	Vout 2	Rich EDC	Rich EDC 2	Heat Out	Recycle	Vinyl Chloride	EDC Recycle	Mix
Vapour Fraction		1,0000	0,0000	0,0000	0,0000	0,0000	1,0000	1,0000	0,7032
Temperature (C)		18,90	18,90	20,24	242,0	-22,36	157,5	40,00	18,90
Pressure (atm)		1,500	1,500	26,00	26,00	9,000	10,00	1,500	1,500
Molar Flow (kgmole/h)		197,8	83,47	83,47	83,47	101,1	48,73	185,4	281,3
Mass Flow (kg/h)		1,091e+004	7587	7587	7587	4541	3045	9173	1,849e+004
Liquid Volume Flow (m ³ /h)		11,46	6,668	6,668	6,668	5,092	3,313	10,19	18,12
Heat Flow (kJ/h)		-9,019e+006	-1,067e+007	-1,065e+007	-6,938e+006	-6,938e+006	2,071e+006	-5,192e+006	-1,969e+007
Name	Unit	Vc 1	Vc 2	Vc 3	EDCa	EDCa Cool	Ethylene	EDC Vapor	EDC Liq 1
Vapour Fraction		1,0000	1,0000	0,8000	0,1684	1,0000	1,0000	1,0000	0,0000
Temperature (C)		250,0	239,9	32,75	-61,26	40,00	25,00	65,00	65,00
Pressure (atm)		25,99	10,00	10,00	2,000	1,500	1,500	1,500	1,500
Molar Flow (kgmole/h)		149,8	149,8	149,8	101,1	101,1	100,0	63,27	41,73
Mass Flow (kg/h)		7587	7587	7587	4541	4541	2580	5787	4109
Liquid Volume Flow (m ³ /h)		8,405	8,405	8,405	5,092	5,092	7,320	5,017	3,482
Heat Flow (kJ/h)		-1,903e+006	-1,903e+006	-4,027e+006	-6,991e+006	-1,117e+006	5,226e+006	-7,117e+006	-6,419e+006
Name	Unit	Cl2	EDC Liq 2	Vapor Out	HCL Rec				
Vapour Fraction		1,0000	0,1435	1,0000	0,0000				
Temperature (C)		25,00	40,00	40,00	40,00				
Pressure (atm)		1,500	1,500	1,500	1,500				
Molar Flow (kgmole/h)		100,0	63,27	9,079	54,91				
Mass Flow (kg/h)		7091	5787	576,1	5211				
Liquid Volume Flow (m ³ /h)		4,541	5,017	0,5598	4,457				
Heat Flow (kJ/h)		-1,181e+004	-8,803e+006	-7,228e+006	-8,080e+006				

Composition	Unit	Vout 2	Rich EDC	Rich EDC 2	Heat Out	Recycle	Vinyl Chloride	EDC Recycle	Mix	Vc 1	Vc 2
Cl2	mole %	1,64E-18	4,34E-19	4,34E-19	4,34E-19	0	0	0	1,29E-18	0	0
Vinyl Chloride	mole %	0,411338	0,192109	0,192109	0,192109	0,343989	0,9999	0,500481	0,348441	0,547322	0,547322
11-ClC2	mole %	0,119653	0,784698	0,784698	0,784698	7,11E-19	2,53E-06	1,89E-14	0,310455	7,84E-07	7,84E-07
HCl	mole %	0,46759	0,023165	0,023165	0,023165	0,65698	9,74E-05	0,499519	0,340081	0,452656	0,452656
Ethylene	mole %	0,001419	3,80E-05	3,80E-05	3,80E-05	3,09E-05	1,22E-11	0	0,001023	2,13E-05	2,13E-05
Composition	Unit	test3	Vc 3	EDCa	EDCa Cool	Ethylene	EDC Vapor	EDC Liq 1	Cl2	EDC Liq 2	Vapor Out
Cl2	mole %	0	0	0	0	0	8,96E-18	8,45E-19	1	8,96E-18	3,08E-17
Vinyl Chloride	mole %	0,999	0,547322	0,343989	0,343989	0	0,055632	0,008333	0	0,055632	0,14788
11-ClC2	mole %	3,92E-10	7,84E-07	7,11E-19	7,11E-19	0	0,852318	0,969798	0	0,852318	0,354519
HCl	mole %	0,001	0,452656	0,65698	0,65698	0	0,057057	0,001346	0	0,057057	0,300817
Ethylene	mole %	0	2,13E-05	3,09E-05	3,09E-05	1	0,034994	0,000524	0	0,034994	0,196683