

Improving Net Energy of Cumene Hydroperoxide Production using Cumene Oxidation Process Through Removing Cooler on the Recycle System to Achieve Energy Efficiency and Reduce Production Cost

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Table S1. Material and heat balance of the modified process

	Unit	Air	Rec	R-Vap	R-Liq	OFFGAS	LF1	V2-VapOut	V2-LiqOut	C2-Out	OFFGAS2	LF2	MIX-OUT	Cumene	P-Out
Total Phase Properties															
Vapour Fraction		1	0	1	0	1	0	1	3,03E-07	3,85E-03	1	0	0	0	0
Temperature	K	333,15	298,0108112	375,41	375,41	293,2	293,2	354,8737839	394,4446281	294,09	294,09	297,992982	333,15	294,349635	
Pressure	atm	2,974	2,974	2,974	2,974	2,974	2,974	9,50E-02	0,11	9,50E-02	9,50E-02	9,50E-02	2,974	2,974	2,974
Mol Weight		28,94197137	119,1029456	34,83303469	121,3681573	28,6711971	115,4608318	118,8455202	146,617211	118,8455202	32,90490696	119,1773181	119,11261	120,194	119,1773181
Molar Flow	kgmole/h	1727,594826	2752,545407	1638,447618	2642,900474	1522,122113	116,3255055	2402,833024	240,0674503	2402,833024	9,241134558	2393,591889	2759,51388	249,59649	2393,591889
Mass Flow	kg/h	50000	327836,2657	57072,10272	320763,9606	43641,0631	13431,03962	285565,9406	35198,02002	285565,9406	304,0786728	285261,8619	328692,902	30000	285261,8619
Heat Flow	kJ/h	1769081,301	-127780944,7	2072717,021	-92202335,7	-957230,857	-7336469,064	18436573,78	-22109732,77	-112649989,8	-27225,05903	-112622765	-128114533	-8283507,2	-112494557
Std Gas Flow	MMSCFD	40848,00605	65082,3849	38740,17056	62489,89227	35989,71954	2750,45102	56813,6327	5676,259569	56813,6327	218,5014186	56595,13128	65247,1505	5901,5682	56595,13128
Vapour Phase Properties															
Mass Flow	kg/h	50000		57072,10272	0	43641,0631	0	285565,9406	9,63E-03	304,0786728	304,0786728	0			
Mol Weight		28,94197137		34,83303469	34,83303469	28,6711971	28,6711971	118,8455202	132,250936	32,90490696	32,90490696	32,90490696			
Mass Density	kg/m ³	3,148611798		3,362918186	3,362918186	3,544154834	3,544154834	0,387723715	0,449464308	0,129537013	0,129537013	0,129537013			
Actual Gas Vol Flow	m ³ /h	15880,01418		16971,00541	0	12313,53176	0	736519,1487	2,14E-02	2347,426937	2347,426937	0			
Compressibility Factor		1		1	1	1	1	1,000000001	1,000000105	1	1	1			
Cp/Cv		1,394875384		1,256899462	1,256899462	1,396227066	1,396227066	1,048673303	1,040667213	1,310209167	1,310209167	1,310209167			
Viscosity	cP	2,05E-02		2,21E-02	2,21E-02	1,84E-02	1,84E-02	6,41E-03	7,19E-03	1,80E-02	1,80E-02	1,80E-02			
Heat Capacity	kJ/kgC	1,014794997		1,167823236	1,167823236	1,021873569	1,021873569	1,507434426	1,608919961	1,067326247	1,067326247	1,067326247			
Thermal Conductivity	W/mK	2,85E-02		2,96E-02	2,96E-02	2,56E-02	2,56E-02	1,41E-02	1,60E-02	2,42E-02	2,42E-02	2,42E-02			
Liquid Phase Properties															
Mass Flow	kg/h	0	327836,2657	0	320763,9606	0	13431,03962	0	35198,01039	285261,8619	0	285261,8619	328692,902	30000	285261,8619
Mol Weight		0	119,1029456	121,3681573	121,3681573	115,4608318	115,4608318	0	146,6172154	119,1773181	119,1773181	119,1773181	119,11261	120,194	119,1773181
Mass Density	kg/m ³	0	862,3439966	819,7744972	819,7744972	876,7137646	876,7137646	0	1082,371792	865,4183475	865,4183475	865,4183475	862,426591	828,47888	865,4348052
Actual Liq Vol Flow	m ³ /s	0	0,105602439	0	0,108689768	0	4,26E-03	0	9,03E-03	9,16E-02	0	9,16E-02	0,10586824	1,01E-02	9,16E-02
Viscosity	cP	0	0,747644609	0,313498487	0,313498487	0,813283013	0,813283013	0	0,446016872	0,788476235	0,788476235	0,788476235	0,74770361	0,4845676	0,785784177
Heat Capacity	kJ/kgC	0	1,746504283	2,055465066	2,055465066	1,725541503	1,725541503	0	2,12212791	1,730341054	1,730341054	1,730341054	1,74643631	1,8906257	1,731409901
Thermal Conductivity	W/mK	0	0,1388955	0,119347282	0,119347282	0,143194718	0,143194718	0	0,104612567	0,139741653	0,139741653	0,139741653	0,13888687	0,129915	0,139680131
Mass Fraction Composition															
Cumene	weight %	0	0,991895305	0,232948004	0,896849244	5,80E-03	0,971016013	0,990869071	0,134054623	0,990869071	0,176197532	0,991737481	0,99164489	1	0,991737481
Oxygen	weight %	0,25761894	2,81E-06	0,112434354	7,97E-05	0,147018842	6,00E-05	8,95E-05	8,72E-26	8,95E-05	8,29E-02	1,25E-06	3,54E-06	0	1,25E-06
Cumene Hydroperoxide	weight %	0	2,22E-03	1,36E-03	9,57E-02	1,68E-08	5,79E-03	2,57E-03	0,851181983	2,57E-03	2,41E-07	2,57E-03	2,47E-03	0	2,57E-03
a,a dimethyl benzyl alcohol	weight %	0	7,68E-05	2,48E-05	1,26E-03	1,08E-08	1,05E-04	9,07E-05	1,07E-02	9,07E-05	2,88E-07	9,08E-05	8,32E-05	0	9,08E-05
Acetophenone	weight %	0	8,64E-05	2,54E-05	5,41E-04	5,29E-08	1,08E-04	1,07E-04	4,06E-03	1,07E-04	1,62E-06	1,07E-04	9,76E-05	0	1,07E-04
Formic Acid	weight %	0	5,60E-03	5,95E-03	4,84E-03	1,23E-03	2,13E-02	5,43E-03	2,52E-07	5,43E-03	9,53E-03	5,43E-03	5,58E-03	0	5,43E-03
Water	weight %	0	8,56E-05	6,35E-04	4,30E-05	5,20E-04	1,01E-03	4,83E-05	1,82E-13	4,83E-05	9,36E-04	4,73E-05	8,23E-05	0	4,73E-05
Mole Fraction Composition															
Cumene	mole %	0	0,982891428	6,75E-02	0,905610429	1,38E-03	0,932777978	0,979752317	0,163524926	0,979752317	4,82E-02	0,983348695	0,98272302	1	0,983348695
Oxygen	mole %	0,233	1,05E-05	0,122388429	3,02E-04	0,131725193	2,17E-04	3,32E-04	4,00E-25	3,32E-04	8,52E-02	4,66E-06	1,32E-05	0	4,66E-06
Cumene Hydroperoxide	mole %	0	1,74E-03	3,12E-04	7,63E-02	3,16E-09	4,39E-03	2,00E-03	0,819997859	2,00E-03	5,22E-08	2,01E-03	1,93E-03	0	2,01E-03
a,a dimethyl benzyl alcohol	mole %	0	6,72E-05	6,35E-06	1,12E-03	2,27E-09	8,94E-05	7,92E-05	1,15E-02	7,92E-05	6,95E-08	7,95E-05	7,27E-05	0	7,95E-05
Acetophenone	mole %	0	8,56E-05	7,36E-06	5,46E-04	1,26E-08	1,04E-04	1,06E-04	4,95E-03	1,06E-04	4,42E-07	1,07E-04	9,67E-05	0	1,07E-04
Formic Acid	mole %	0	1,45E-02	4,50E-03	1,27E-02	7,65E-04	5,34E-02	1,40E-02	8,04E-07	1,40E-02	6,81E-03	1,41E-02	1,44E-02	0	1,41E-02
Water	mole %	0	5,66E-04	1,23E-03	2,89E-04	8,28E-04	6,47E-03	3,18E-04	1,48E-12	3,18E-04	1,71E-03	3,13E-04	5,44E-04	0	3,13E-04
Total	mole %		1	1	1	1	1	1	1	1	1	1	1	1	1