

Optimization of Acetic Acid Production Process Using the Cativa Method for Increasing Product Purity

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Table S1. Heat and material balances for basic Cativa process

Energy stream				
		Q-100	QC 8	QR 9
Heat Flow	kJ/h	2.584e+006	2.022e+005	7.995e+005

Material Streams												
		Carbon monoxide	Methanol	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Stream 8	Stream 9
Vapour Fraction		1.000	0.0000	1.0000	0.0000	1.0000	0.0000	0.3521	1.0000	0.0000	1.0000	0.0000
Temperature	C	30.000	30.00	634.2	634.2	453.4	453.4	30.00	30.00	30.00	97.39	138.5
Pressure	atm	1.000	1.000	1.000	1.000	1.000	1.000	0.9869	0.9869	0.9869	3.000	2.961
Molar Flow	kgmole/h	35.70	31.21	40.38	0.0000	46.25	0.0000	46.25	16.28	29.96	5.954	24.01
Mass Flow	kg/h	1000	1000	2000	0.0000	2000	0.0000	2000	468.3	1532	190.7	1341
Liquid Volume Flow	m3/h	1.251	1.251	2.025	0.0000	2.132	0.0000	2.132	0.5815	1.550	0.2397	1.310
Heat Flow	kJ/h	-3.943e+006	-7.531e+00e	-1.147e+007	-0.0000	-1.147e+007	-0.0000	-1.406e+007	-1.972e+006	-1.209e+007	-1.180e+006	-1.031e+007

Compositions											
	Carbon Monoxide	Methanol	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Stream 8	Stream 9
Comp Mole Frac (Methanol)	0.0000	1.0000	0.1159	0.1159	0.2280	0.2280	0.2280	0.0814	0.3186	0.9986	0.1500
Comp Mole Frac (CO)	1.0000	0.0000	0.2271	0.2271	0.3252	0.3252	0.3252	0.9230	0.0003	0.0014	0.0000
Comp Mole Frac (Acetic Acid)	0.0000	0.0000	0.6569	0.6569	0.4468	0.4468	0.4468	0.0156	0.6811	0.0000	0.8500

Table S2. Heat and material balance for Cativa process after modification

Energy Streams													
		Q-100	Q-101	Q-102	Q-103	Q-104	QC	QR	Q-105				
Heat Flow	kJ/h	1.776e+006	1.325e+007	0.0000	1.523e+006	6.931e+005			1.040e+007				
		Q-106	QC 11	QR 12	Q-107	Q-108	Q-109	Q-110					
Heat Flow	kJ/h	1.010e+007	2.204e+006	1.459e+006	5.179e+005	0.0000	5.500e+005	0.0000					

Material Streams													
		Carbon Monoxide	Methanol	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Stream 8	11	12	Stream 9
Vapour Fraction		1.0000	0.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	1.0000			1.0000
Temperature	C	30.00	30.00	150.0	969.0	30.00	200.0	531.7	907.4	1081			568.8
Pressure	atm	1.000	1.000	1.000	30.00	1.000	1.000	30.00	30.00	30.00	3.000	3.000	1.000
Molar Flow	kgmole/h	35.70	31.21	503.00	503.00	31.21	31.21	31.21	534.2	503.0			503.0
Mass Flow	kg/h	1000	1000	1.410e+004	1.410e+004	1000	1000	1000	1.510e+004	1.510e+004			1.510e+004
Liquid Volume Flow	m3/h	1251	1257	17.63	17.63	1.257	1.257	1.257	18.89	18.32			18.32
Heat Flow	kJ/h	-3.943e+006	-7.531e+006	-5.387e+007	-4.061e+007	-7.531e+006	-6.008e+006	-5.315e+006	-4.593e+007	-4.593e+007			-5.633e+007
		Stream 10	Stream 11	Stream 12	Stream 15	Stream 16	Stream 17	Stream 18	Stream 13	Stream 14	Stream 19	Stream 1	
Vaour Fraction		0.9665	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	1.0000	1.0000	1.0000	1.0000	
Temperature	C	35.00	-9.817	156.2	35.00	35.00	35.00	35.00	30.00	30.00	30.00	29.48	
Pressure	atm	1.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	1.000	
Molar Flow	kgmole/h	503.0	471.8	31.21	31.21	31.21	0.0000	31.21	471.8	471.8	467.3	503.0	
Mass Flow	kg/h	1.510e+004	1.322e+004	1874	1874	1874	0.0000	1874	1.322e+004	1.322e+004	1.310e+004	1.410e+004	
Liquid Volume Flow	m3/h	18.32	16.54	1.782	1.782	1.782	0.0000	1.782	16.54	16.54	16.38	17.63	
Heat Flow	kJ/h	-6.643e+007	-5.275e+007	-1.443e+007	-1.495e+007	-1.495e+007	0.0000	-1.495e+007	-5.220e+007	-5.220e+007	-5.170e+007	-5.564+007	

Compositions												
	Carbon Monoxide	Methanol	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Stream 8	11	12	Stream 9
Comp Mole Fraction (Methanol)	0.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0584	0.0000			0.0000
Comp Mole Fraction (H ₂ O)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000			0.0000
Comp Mole Fraction (CO)	1.0000	0.0000	0.9995	0.9995	0.0000	0.0000	0.0000	0.9411	0.9375			0.9375
Comp Mole Fraction (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000			0.0000
Comp Mole Fraction (Acetic Acid)	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0004	0.0625			0.0625
Comp Mole Fraction (M-Acetate)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000			0.0000
	Stream 10	Stream 11	Stream 12	Stream 15	Stream 16	Stream 17	Stream 18	Stream 13	Stream 14	Stream 19	Stream 1	
Comp Mole Fraction (Methanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Comp Mole Fraction (H ₂ O)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Comp Mole Fraction (CO)	0.9375	0.9995	0.0000	0.0000	0.0000	0.0000	0.0000	0.9995	0.9995	0.9995	0.9995	
Comp Mole Fraction (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Comp Mole Fraction (Acetic Acid)	0.0625	0.0005	1.0000	1.0000	1.0000	1.0000	1.0000	0.0005	0.0005	0.0005	0.0000	
Comp Mole Fraction (M-Acetate)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	