

Supplementary Information

Classical and Process Intensification Methods for Acetic Acid Concentration: Technical and Environmental Assessment

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The main input and output streams correspondent to each case under study are summarized in Tables S1–S5. The cases investigated are:

Case 1 - Acetic acid concentration using ethyl acetate;

Case 2 - Acetic acid concentration using isopropyl acetate;

Case 3 - Acetic acid concentration using isopropyl acetate and isopropanol mixture;

Case 4 - Acetic acid concentration using isopropyl acetate and isopropanol mixture by TC;

Case 5 - Acetic acid concentration using isopropyl acetate and isopropanol mixture by DED.

Table S1. Main streams for Case 1.

Stream	Unit	S1	S2	S3	S5	S9	S12	S13
Temperature	° C	25.00	25.00	25.00	116.42	25.00	100.00	102.50
Pressure	kPa	101.33	101.33	101.33	101.33	101.33	101.33	101.33
Vapor fraction	-	0.00	0.00	0.00	0.00	0.00	1.00	0.00
Component flow-rate								
Water	kmol/h	861.00	176.53	400.15	7.06	661.39	18.37	896.31
Acetic acid		139.00	22.11	130.58	106.34	6.53	0.00	8.66
Ethyl Acetate		0.00	740.00	731.45	9.20x10 ⁻¹⁸	8.55	0.00	0.00
Total mole flow-rate	kmol/h	1000.00	938.64	1261.18	113.40	676.47	18.37	904.97

Table S2. Main streams for Case 2.

Stream	Unit	S1	S3	S4	S5	S12	S19	S20
Temperature	° C	150.00	90.00	70.84	120.65	96.76	71.22	76.38
Pressure	kPa	500.00	200.00	110.00	110.00	110.00	250.00	110.00
Vapor fraction	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Component flow-rate								
Water	kmol/h	861.00	220.83	692.49	1.42x10 ⁻⁷	862.34	17.79	124.01
Acetic acid		139.00	134.93	4.10	134.93	4.10	1.35x10 ⁻⁸	7.87x10 ⁻⁸
Isopropyl acetate		0.00	338.73	4.42	0.14	0.15	4.90	337.96
Total mole flow-rate	kmol/h	1000.00	694.49	701.01	135.07	866.59	22.69	461.97

Table S3. Main streams for Case 3.

Stream	Unit	S1	S3	S4	S5	S12	S19	S20
Temperature	° C	150.00	90.00	70.77	120.65	96.67	73.34	76.44
Pressure	kPa	500.00	200.00	200.00	110.00	110.00	250.00	110.00
Vapor fraction	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Component flow-rate								
Water	kmol/h	861.00	224.81	688.51	1.46x10 ⁻⁷	861.41	17.98	126.21
Acetic acid		139.00	135.41	3.63	135.41	3.62	1.06x10 ⁻⁸	1.06x10 ⁻⁸
Isopropanol		0.00	3.40	1.10	1.00x10 ⁻⁴	1.49x10 ⁻³	1.10	3.39
Isopropyl acetate		0.00	338.71	4.43	0.14	0.15	5.19	337.66
Total mole flow-rate	kmol/h	1000.00	702.33	697.67	135.55	865.18	24.27	467.26

Table S4. Main streams for Case 4.

Stream	Unit	S1	S3	S4	S5	S9	S10	S14
Temperature	° C	150.00	92.11	70.00	141.28	119.97	99.82	70.00
Pressure	kPa	500.00	200.00	200.00	198.00	198.00	198.00	200.00
Vapor fraction	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Component flow-rate								
Water	kmol/h	861.00	235.25	689.87	1.02x10 ⁻⁶	818.19	65.83	106.94
Acetic acid		139.00	138.99	0.04	134.05	4.98	1.22	9.71x10 ⁻³
Isopropanol		0.00	4.46	1.08	1.18x10 ⁻⁴	3.00x10 ⁻⁹	2.03	5.52
Isopropyl acetate		0.00	416.40	4.15	2.35x10 ⁻²	0.00	64.89	420.53
Total mole flow-rate	kmol/h	1000.00	795.10	695.11	134.07	823.17	133.97	532.99

Table S5. Main streams for Case 5.

Stream	Unit	S1	S4	S5	S12	S14	S15	S18	S20
Temperature	°C	150	118.50	162.37	114.35	74.84	114.25	101.78	169.29
Pressure	kPa	500	340.00	340.00	340.00	110.00	340.00	110.00	100.00
Vapor fraction	-	0.00	0.16	0.00	0.93	0.00	0.93	0.41	0.00
Component flow-rate									
Water	kmol/h	861.00	296.69	0.15	138.92	51.42	157.63	890.68	678.88
Acetic acid		139.00	136.51	135.86	0.30	1.08x10 ⁻⁶	0.35	3.18	2.88
Isopropanol		0.00	34.31	5.28x10 ⁻⁸	16.07	26.74	18.24	4.83	15.49
Isopropyl acetate		0.00	244.85	2.72x10 ⁻¹³	114.69	121.84	130.14	3.15	10.29
Total mole flow-rate	kmol/h	1000.00	712.36	136.01	269.98	200.00	306.36	901.84	707.54