Supporting information to article

Reaction-separation-recycle processes for *2*-ethylhexyl acrylate production: Design, control and economic evaluation

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Experimental data retrieved from literature[1]

Table S1 – Experimental data of 2-EHA mole fraction as function of temperature read from Fig.7 and Fig.8 from the paper of Komon et al. (2013)[1]. Data retrieved with permission from the original reference[1]. Copyright 2013 Elsevier.

Data read from Fig.7 [1]												
AA : *2*-EH	1:7				1:5				1:3			
T / [K]	363	373	383	393	363	373	383	393	363	373	383	393
Time ↓	*2*-EHA mole fraction											
0	0	0	0	0	0	0	0	0	0	0	0	0
15	0.0067	0.0111	0.0177	0.0419	0.0134	0.0205	0.0353	0.0482	0.0187	0.0278	0.0472	0.0512
30	0.0115	0.0284	0.0441	0.0649	0.0187	0.0408	0.0600	0.0837	0.0333	0.0538	0.0842	0.1145
45	0.0256	0.0441	0.0610	0.0832	0.0313	0.0582	0.0855	0.1053	0.0512	0.0765	0.1123	0.1548
60	0.0300	0.0532	0.0766	0.0959	0.0426	0.0761	0.1021	0.1197	0.0622	0.0962	0.1416	0.1760
80	0.0429	0.0653	0.0846	0.1035	0.0542	0.0890	0.1190	0.1392	0.0834	0.1244	0.1592	0.1983
100	0.0494	0.0751	0.0967	0.1104	0.0700	0.0990	0.1287	0.1447	0.0976	0.1397	0.1774	0.2067
120	0.0600	0.0850	0.1015	0.1136	0.0800	0.1132	0.1363	0.1508	0.1112	0.1555	0.1847	0.2148
150	0.0693	0.0923	0.1094	0.1166	0.0924	0.1234	0.1450	0.1550	0.1360	0.1723	0.2016	0.2177
180	0.0794	0.1011	0.1150	0.1162	0.1045	0.1350	0.1513	0.1576	0.1488	0.1803	0.2052	0.2297
210	0.0850	0.1078	0.1172	0.1176	0.1129	0.1440	0.1534	0.1582	0.1550	0.1909	0.2121	0.2322
240	0.0913	0.1090	0.1182	0.1189	0.1200	0.1487	0.1545	0.1595	0.1715	0.2037	0.2179	0.2373
300	0.1017	0.1150	0.1191	0.1195	0.1308	0.1513	0.1600	0.1600	0.1824	0.2131	0.2267	0.2387
360	0.1078	0.1176	0.1182	0.1201	0.1379	0.1547	0.1592	0.1595	0.1948	0.2186	0.2273	0.2358
Data read from Fig.8 of reference [1]												
AA : *2*-EH	3:1				5:1				7:1			
T / [K]	353	363	373	383	353	363	373	383	353	363	373	383
Time ↓	*2*-EHA mole fraction											
0	0	0	0	0	0	0	0	0	0	0	0	0
15	0.0137	0.0189	0.0335	0.0644	0.0145	0.0326	0.0296	0.0456	0.0123	0.0214	0.0272	0.0353
30	0.0232	0.0356	0.0640	0.0910	0.0196	0.0372	0.0507	0.0716	0.0163	0.0284	0.0422	0.0551
45	0.0339	0.0506	0.0850	0.1180	0.0293	0.0500	0.0688	0.0913	0.0228	0.0383	0.0555	0.0716
60	0.0451	0.0652	0.1060	0.1373	0.0375	0.0625	0.0816	0.1084	0.0294	0.0476	0.0658	0.0833
80	0.0575	0.0871	0.1240	0.1558	0.0469	0.0757	0.0948	0.1209	0.0373	0.0571	0.0760	0.0930
100	0.0704	0.0957	0.1391	0.1695	0.0548	0.0869	0.1061	0.1300	0.0438	0.0647	0.0851	0.0999
120	0.0798	0.1116	0.1528	0.1798	0.0620	0.0971	0.1101	0.1359	0.0498	0.0720	0.0924	0.1051
150	0.0927	0.1150	0.1644	0.1919	0.0722	0.1048	0.1265	0.1425	0.0587	0.0807	0.0988	0.1099
180	0.1039	0.1335	0.1760	0.1991	0.0816	0.1165	0.1308	0.1446	0.0656	0.0869	0.1037	0.1130
210	0.1137	0.1425	0.1858	0.2069	0.0892	0.1229	0.1369	0.1497	0.0720	0.0912	0.1075	0.1126
240	0.1228	0.1558	0.1923	0.2086	0.0961	0.1285	0.1410	0.1489	0.0758	0.0978	0.1101	0.1126
300	0.1373	0.1648	0.2000	0.2150	0.1066	0.1374	0.1469	0.1474	0.0837	0.1025	0.1140	0.1186
360	0.1485	0.1858	0.2069	0.2142	0.1155	0.1418	0.1502	0.1471	0.0906	0.1085	0.1164	0.1166

Tuning parameters of the RSR-A, RSR-B, and RSR-C processes

Table S2 – Tuning parameters of the RSR-A process

Controllers	*Process value (PV)*		*Controller output (OP)*		K_C	T_i
	Value	*Range*	*Value*	*Range*	*%/%*	*min*
Plantwide inventory						
X ($F_1/F_{AA,0}$)	Fresh AA flow rate / kg/h		Recycle+Fresh *2*-EH flow rate / kg/h		-	-
	$F_1 = 9.09 \times F_{AA,0}$					
V-1						
LC	Level / m		Flow rate / kg/h		10	60
	0.65	0…1.3	1778.9	0 … 3557.9		
PFR & HX-1						
TC	Temperature (inlet PFR) / °C		Duty / GJ/h		1	20
	120	95…145	-0.8889	0 … 2.6667		
C-1 & COND-1						
PC	Pressure (tray 1) / bar		Flow rate / m^3/h		2	12
	0.1	0.08…0.12	448.2	0 … 1345.5		
TC	Temperature (tray 8) / °C		Duty / GJ/h		1.459	9.24
	83.2	73.2 … 93.2	1.0282	0 … 2.26		
LC	Level / m		Flow rate / kg/h		1	60
	0.675	0 … 1.35	8647.2	0 … 17294.4		
TC	Temperature (condenser) / °C		Duty / GJ/h		1	20
	30	20…40	-1.0213	-2.0425… 0		
V-2						
LC	Level (organic) / m		Flow rate / kg/h		1	60
	0.225	0…0.65	40.4	0 … 122.9		
LC	Level (aqueous) / m		Flow rate / kg/h		1	60
	0.21	0…0.45	407.9	0 … 1222.7		
C-2, COND-2 & V-3						
PC	Pressure (condenser) / bar		Condenser Duty / GJ/h		2	12
	0.1	0.08…0.12	-7.6224	-14.3408… 0		
TC	Temperature (tray 22) / °C		Duty / GJ/h		0.1	11.88
	147.3	137.3…157.3	7.6	0…14.26		
LC	Level (reflux drum) / m		Flow rate / kg/h		1	60
	1.66	0…3.33	6135.3	0…12271		
LC	Level (sump) / m		Flow rate / kg/h		1	60
	1	0…2	2511.9	0 … 5023.8		
TC	Temperature (*2*-EHA cooling) / °C		Duty / GJ/h		1	20
	30	20…40	-0.6463	-1.293 … 0		

Concentration controller (QC) and Analyzer (A)						
QC	(AA + *2*-EH) / [kg/kg]		Temperature / [°C]		0.086	43.56
	5	0 … 10	147.3	127.3 … 167.3		
A_1	Input_1 = 4.840 x 10^{-6} AA mass fraction / [kg/kg]		Output_1 = 4.840 x 10^{-3} AA transf. mass frac. / [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					
A_2	Input_2 = 4.984 x 10^{-3} *2*-EH mass fraction / [kg/kg]		Output_2 = 4.984 *2*-EH transf. mass frac./ [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					

Table S3 – Tuning parameters of the RSR-B process

Controllers	*Process value (PV)*		*Controller output (OP)*		K_C	T_i
	Value	*Range*	*Value*	*Range*	*%/%*	*min*
Plantwide inventory						
X (F_1 /$F_{AA,0}$)	Fresh AA flow rate / kg/h		Recycle+Fresh *2*-EH flow rate / kg/h		-	-
	$F_1 = 8.45 \times F_{AA,0}$					
V-1						
LC	Level / m		Flow rate / kg/h		10	60
	0.79	0 … 1.3	1762	0 … 3524		
PFR & HX-1						
TC	Temperature (inlet PFR) / °C		Duty / GJ/h		1	20
	120	95 … 145	-1.03614	0 … 3.26249		
V-4 & COND-1						
PC	Pressure / bar		Flow rate / m^3/h		2	12
	0.15	0.13 … 0.17	586.5	0 … 1759.5		
LC	Level / m		Flow rate / kg/h		1	60
	0.6	0 … 1.2	8654.5	0 … 17308.9		
TC	Temperature (condenser) / °C		Duty / GJ/h		1	20
	30	20 … 40	-0.84189	-1.68398 … 0		
V-2						
LC	Level (organic) / m		Flow rate / kg/h		1	60
	0.79	0 … 1.35	334.6	0 … 1003.8		
LC	Level (aqueous) / m		Flow rate / kg/h		1	60
	0.34	0 … 1.35	251.8	0 … 755.7		
C-2, COND-2 & V-3						
PC	Pressure (condenser) / bar		Condenser Duty / GJ/h		2	12
	0.1	0.08…0.12	-8.98934	-17.98288 … 0		
TC	Temperature (tray 22) / °C		Duty / GJ/h		0.084	13.86
	147.3	137.3 … 157.3	9.06477	0 … 18.13411		
LC	Level (reflux drum) / m		Flow rate / kg/h		1	60

	1.3	0 … 2.55	6501.2	0 … 13002.7		
LC	Level (sump) / m		Flow rate / kg/h		1	60
	1.1	0 … 2.2	2488	0 … 4975.4		
TC	Temperature (*2*-EHA cooling) / °C		Duty / GJ/h		1	20
	30	20…40	-0.64025	-1.28042 … 0		
Concentration controller (QC) and Analyzer (A)						
QC	(AA + *2*-EH) / [kg/kg]		Temperature / [°C]		0.092	44.22
	5	0 … 10	147.3	127.3 … 167.3		
A_1	Input_1 = 4.717 x 10^{-6} AA mass fraction / [kg/kg]		Output_1 = 4.717 x 10^{-3} AA transf. mass frac. / [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					
A_2	Input_2 = 4.990 x 10^{-3} *2*-EH mass fraction / [kg/kg]		Output_2 = 4.990 *2*-EH transf. mass frac./ [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					

Table S4 – Tuning parameters of the RSR-C process

Controllers	*Process value (PV)*		*Controller output (OP)*		K_C	T_i
	Value	*Range*	*Value*	*Range*	*%/%*	*min*
Plantwide inventory						
X (F_1 /$F_{AA,0}$)	Fresh AA flow rate / kg/h		Recycle+Fresh *2*-EH flow rate / kg/h		-	-
	$F_1 = 10.2 \times F_{AA,0}$					
V-1						
LC	Level / m		Flow rate / kg/h		10	60
	0.7	0 … 1.4	1765	0 … 3530		
PFR & HX-1						
TC	Temperature (inlet PFR) / °C		Duty / GJ/h		1	20
	120	95 … 145	-2.51937	0 … 5.0383		
V-2						
LC	Level (organic) / m		Flow rate / kg/h		1	60
	1.83	0 … 3.65	10703	0 … 21406		
LC	Level (aqueous) / m		Flow rate / kg/h		10	60
	0.5	0 … 3.65	250.5	0 … 735		
C-2, COND-2 & V-3						
PC	Pressure (condenser) / bar		Condenser Duty / GJ/h		2	12
	0.1	0.08…0.12	-11.3535	-22.7142 … 0		
TC	Temperature (tray 34) / °C		Duty / GJ/h		0.082	13.2
	154.5	144.5 … 164.5	12.4208	0 … 24.8492		
LC	Level (reflux drum) / m		Flow rate / kg/h		1	60
	1.25	0 … 2.55	8210.6	0 … 16421.3		
LC	Level (sump) / m		Flow rate / kg/h		1	60

	1.25	0 … 2.5	2493	0 … 4984		
TC	Temperature (*2*-EHA cooling) / °C		Duty / GJ/h		1	20
	30	20…40	-0.63656	-1.36738 … 0		
Concentration controller (QC) and Analyzer (A)						
QC	(AA + *2*-EH) / [kg/kg]		Temperature / [°C]		0.1	54.78
	5	0 … 10	154.5	134.5 … 174.5		
A_1	Input_1 = 3.429 x 10^{-6} AA mass fraction / [kg/kg]		Output_1 = 3.429 x 10^{-3} AA transf. mass frac. / [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					
A_2	Input_2 = 4.987 x 10^{-3} *2*-EH mass fraction / [kg/kg]		Output_2 = 4.987 *2*-EH transf. mass frac./ [kg/kg]		-	-
	Settings: Sensor Gain = 1000; Sample interval = 30 min; Dead time = 30 min					

Calculation of the Total Capital Investment (C_{TCI}) from the Total Installed Cost (C_{TBM}) of process equipment

Given the C_{TBM}, the calculation of C_{TCI} is calculated using some selected factors for various other costs. The selected factors and their justification are given in the following table.

Table S5 – Selected cost factors, their justification, and the resulting costs; based upon the adjusted Guthrie method as described by Seider et al. [2]

Short description	Symbol	Factor	Cost / [$]	Justification
Total bare-module (total installed)	C_{TBM}		1 837 306	
Site preparation	C_{site}	0.05	91 865	Addition to an existing site
Process and non-process buildings	$C_{buildings}$	0.05	91 865	Non-process; integrated site
Utility plants†	$C_{offsite\ facilities}$	0	0	Purchased; no upgrades required
Contingency and contractor fee‡		0.18	363 787	Typical value
Total Permanent Investment₸	C_{TPI}		2 384 823	
Working capital	C_{WC}	0.176	419 729	Typical value
Royalties	C_{royal}	0	0	No licensing fees
Start-up	$C_{startup}$	0.1	238 482	Typical value
Total Capital Investment§	$\boldsymbol{C_{TCI}}$		**3 043 035**	

Notes
† - energy, pollution control, ponds, waste treatment, offsite tankage, and receiving and shipping facilities
‡ - not explicitly showed in Equation ***Error! Reference source not found.****, but taken into consideration by the 0.18 factor (= 1.18 – 1), as factor of the Total Permanent Investment, C_{TPI}; 0.18 is formed from 0.15 contingency, and 0.03 contractor fee*
₸ - sum of costs using factors applied to C_{TBM}, and addition of C_{TBM}
§ - sum of costs using factors applied to C_{TPI}, and addition of C_{TPI}

References

1. Komon, T.; Niewiadomski, P.; Oracz, P.; Jamroz, M. E., Esterification of acrylic acid with *2*-ethylhexan-*1*-ol: Thermodynamic and kinetic study. *Applied Catalysis a-General* **2013**, *451*, 127-136.
2. Seider, W. D.; Seader, J. D.; Lewin, D. R.; Widagdo, S., Product and Process Design Principles. 3rd Edition, International Student Version; John Wiley & Sons, 2010.