Supporting Information

The Impact of Feed Composition on Entrainer Selection in the Extractive Distillation Process
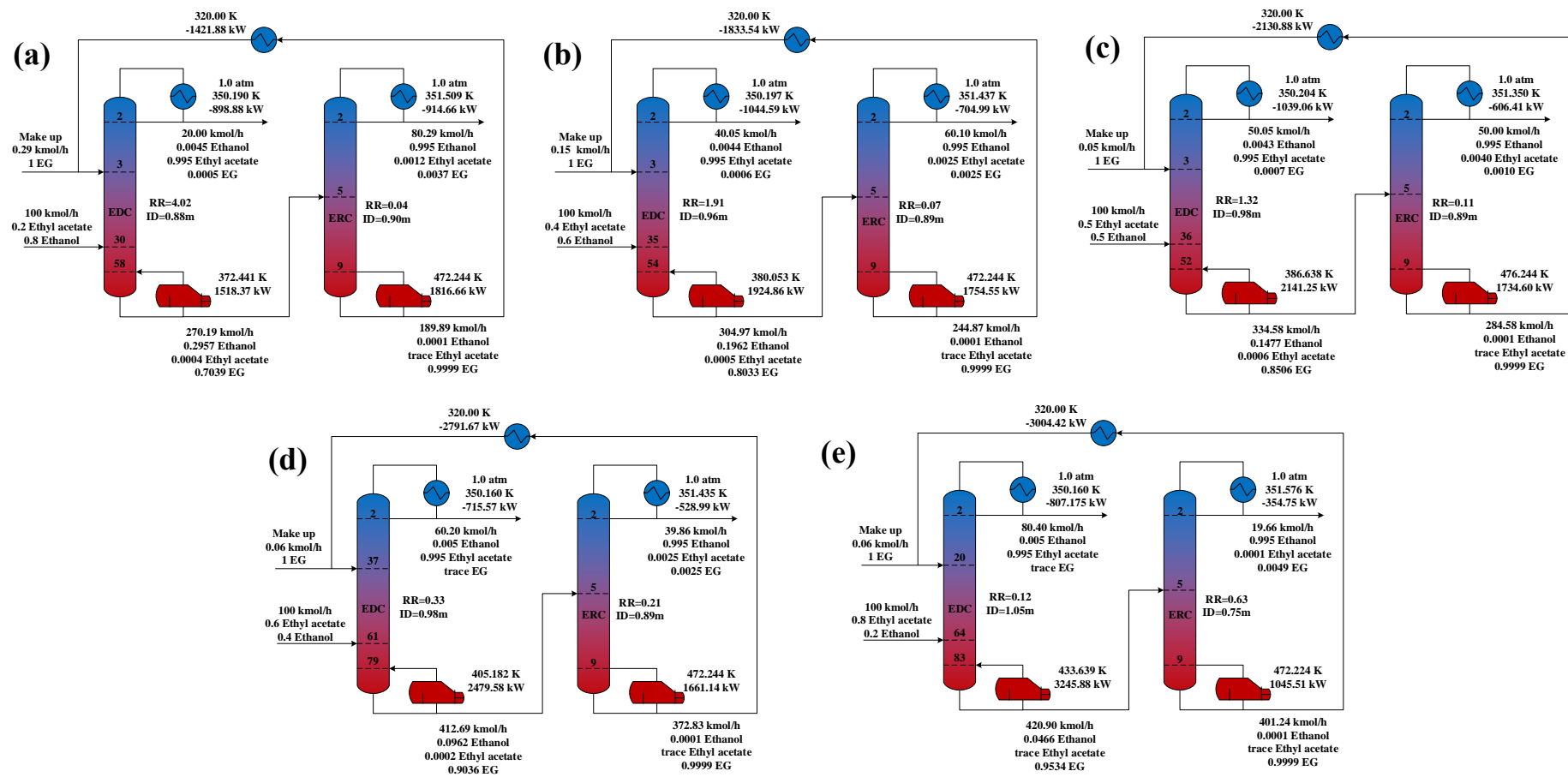
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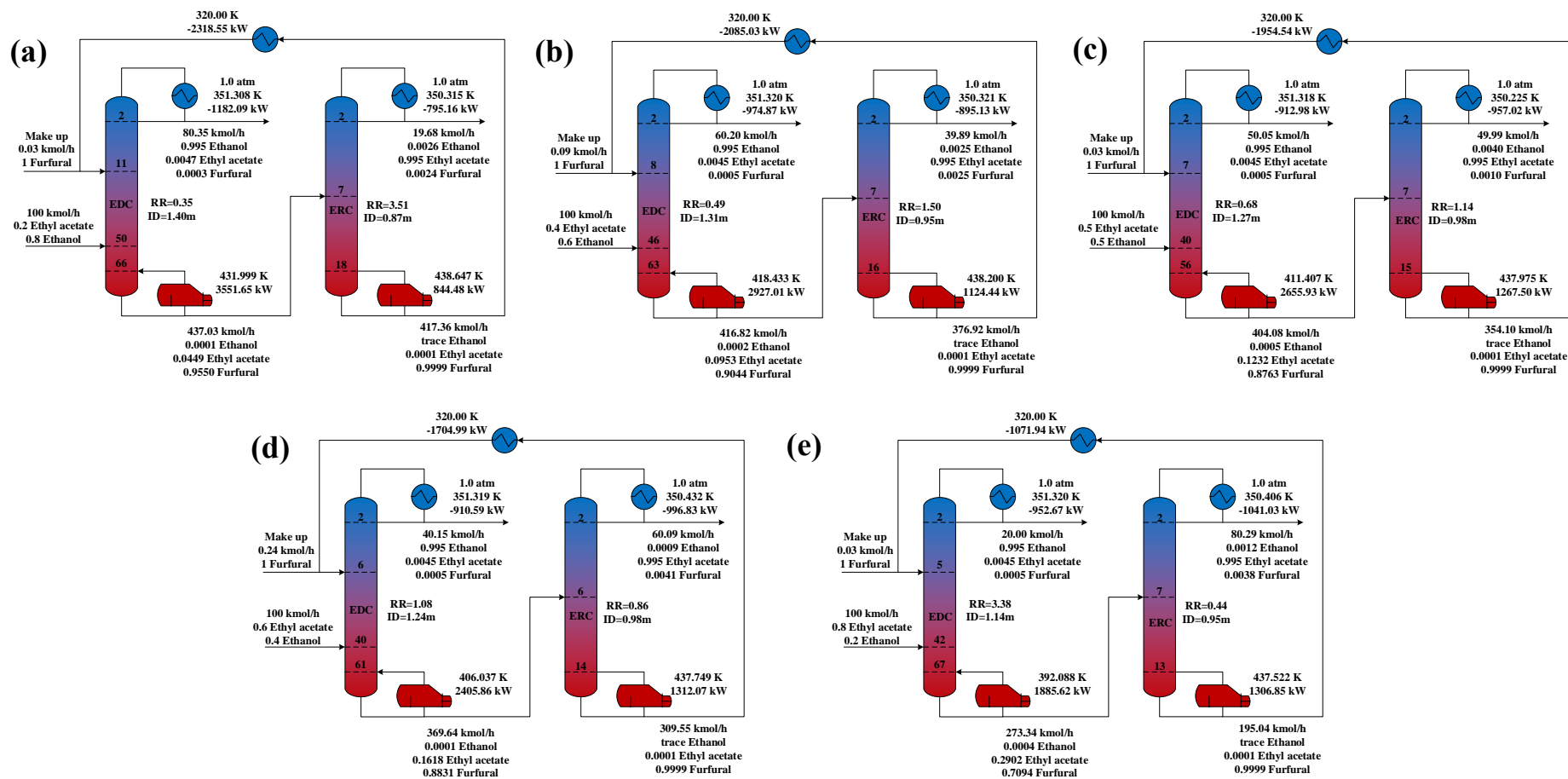
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Figure S1 Optimization results of extractive distillation schemes using EG as the entrainer with stream information for separating ethyl acetate-ethanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

Figure S2 Optimization results of extractive distillation schemes using furfural as the entrainer with stream information for separating ethyl acetate-ethanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

(a)

320.00 K
-167.516 kW

1.0 atm
329.296 K
-864.648 kW

20.00 kmol/h
0.995 Acetone
0.004 Methanol
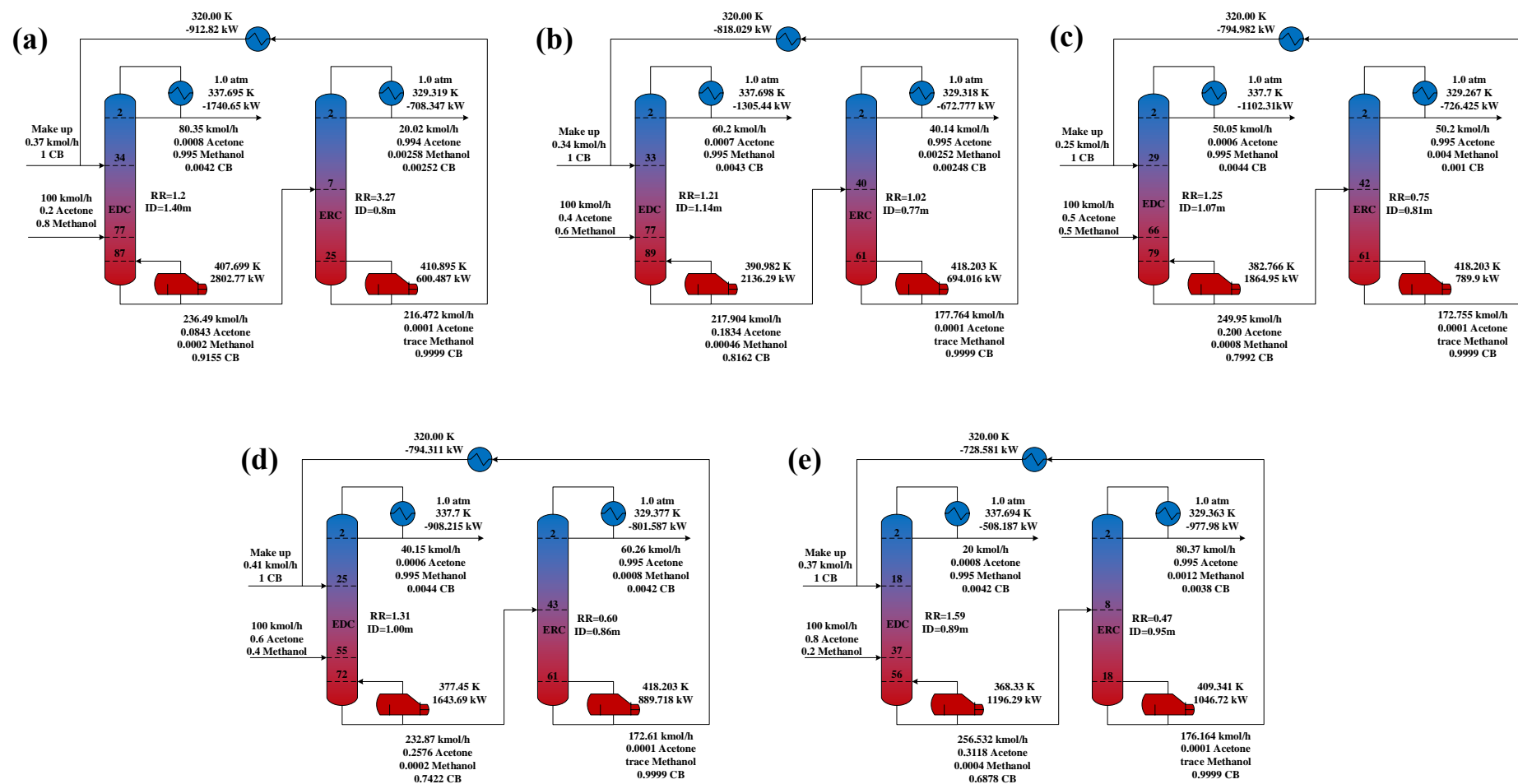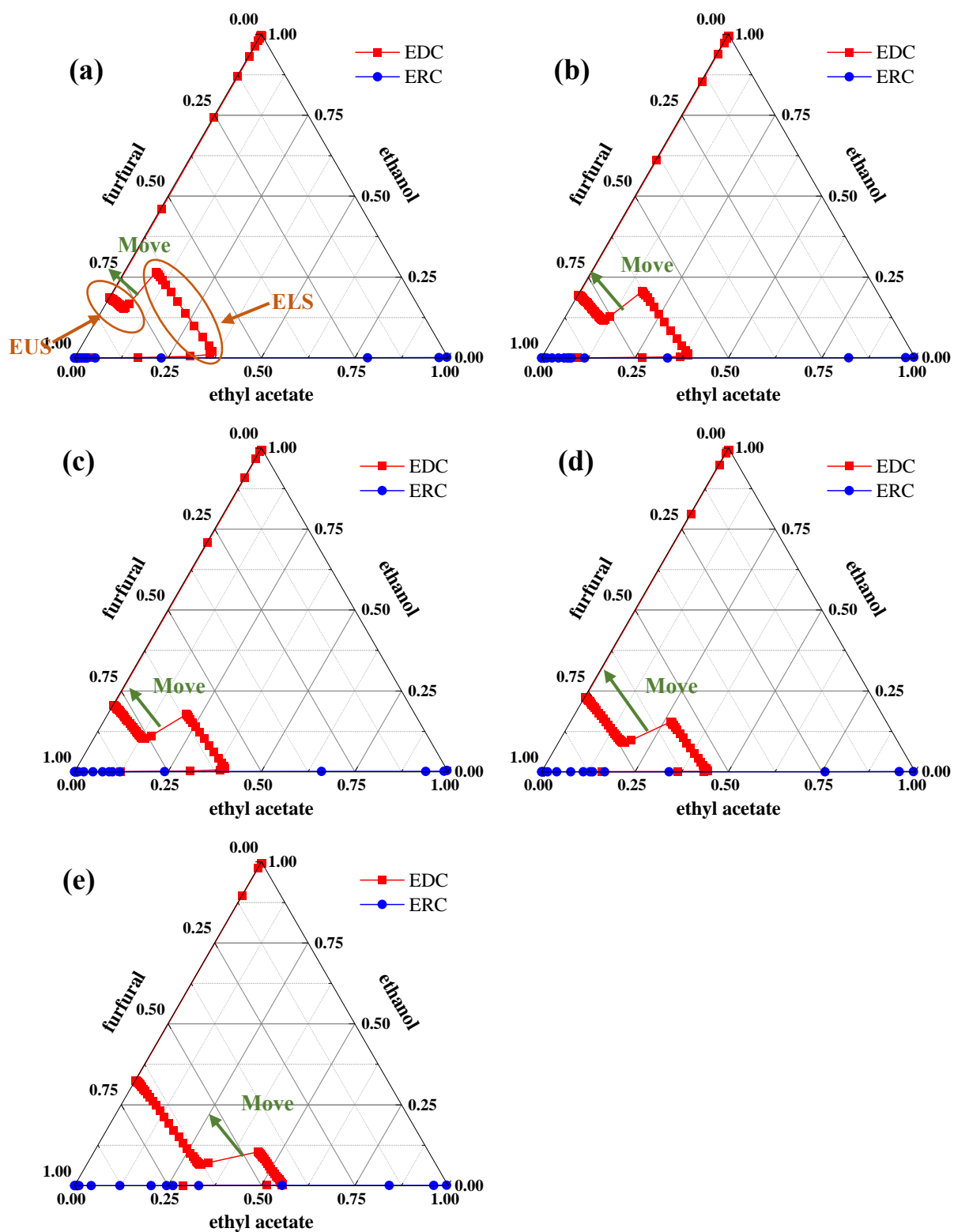0.001 water

Make up
0.37 kmol/h
1 water

100 kmol/h
0.2 Acetone
0.8 Methanol

EDC
RR=4.24
ID=0.79m

357.662 K
1036.9 kW

210.684 kmol/h
0.00047 Acetone
0.3796 Methanol
0.6199 water

1.0 atm
337.696 K
-1555.32 kW

80.37 kmol/h
0.001 Acetone
0.995 Methanol
0.004 water

ERC
RR=0.97
ID=0.86m

378.536 K
1593.18 kW

130.315 kmol/h
trace Acetone
0.0001 Methanol
0.9999 water

(b)

320.00 K
-200.661 kW

1.0 atm
329.3 K
-1194.62 kW

40.05 kmol/h
0.9947 Acetone
0.0009 Methanol
0.0044 water

Make up
0.3 kmol/h
1 water

100 kmol/h
0.4 Acetone
0.6 Methanol

EDC
RR=2.61
ID=0.92m

361.893 K
1396.43 kW

216.35 kmol/h
0.0007 Acetone
0.277 Methanol
0.722 water

1.0 atm
337.622 K
-1255.49 kW

60.25 kmol/h
0.0027 Acetone
0.995 Methanol
0.0023 water

ERC
RR=1.13
ID=0.78m

378.536 K
1289.84 kW

156.1 kmol/h
trace Acetone
0.0001 Methanol
0.9999 water

(c)

320.00 K
-204.326 kW

1.0 atm
329.303 K
-1430.98 kW

50.05 kmol/h
0.995 Acetone
0.00057 Methanol
0.00443 water

Make up
0.26 kmol/h
1 water

100 kmol/h
0.5 Acetone
0.5 Methanol

EDC
RR=2.46
ID=1.01m

364.424 K
1641.94 kW

208.704 kmol/h
0.001 Acetone
0.24 Methanol
0.759 water

1.0 atm
337.555 K
-1098.89kW

50.21 kmol/h
0.004 Acetone
0.995 Methanol
0.001 water

ERC
RR=1.23
ID=0.73m

378.695 K
1125.23 kW

158.497 kmol/h
trace Acetone
0.0001 Methanol
0.9999 water

(d)

320.00 K
-225.832 kW

1.0 atm
329.302 K
-1701.4 kW

60.2 kmol/h
0.995 Acetone
0.00065 Methanol
0.00435 water

Make up
0.34 kmol/h
1 water

100 kmol/h
0.6 Acetone
0.4 Methanol

EDC
RR=2.42
ID=1.1m

367.279 K
1938.19 kW

217.37 kmol/h
0.0005 Acetone
0.1838 Methanol
0.8157 water

1.0 atm
337.63 K
-964.921 kW

40.14 kmol/h
0.0025 Acetone
0.995 Methanol
0.0025 water

ERC
RR=2.35
ID=0.68m

378.049 K
985.304 kW

177.226 kmol/h
trace Acetone
0.0001 Methanol
0.9999 water

(e)

320.00 K
-284.998 kW

1.0 atm
329.303 K
-2237.85 kW

80.4 kmol/h
0.995 Acetone
0.0006 Methanol
0.0044 water

Make up
0.43 kmol/h
1 water

100 kmol/h
0.8 Acetone
0.2 Methanol

EDC
RR=2.37
ID=1.27m

375.083 K
2556.21 kW

244.347 kmol/h
trace Acetone
0.082 Methanol
0.918 water

1.0 atm
337.756 K
-735.56 kW

20.03 kmol/h
0.0001 Acetone
0.995 Methanol
0.0049 water

ERC
RR=2.74
ID=0.59m

377.885 K
733.311 kW

224.32 kmol/h
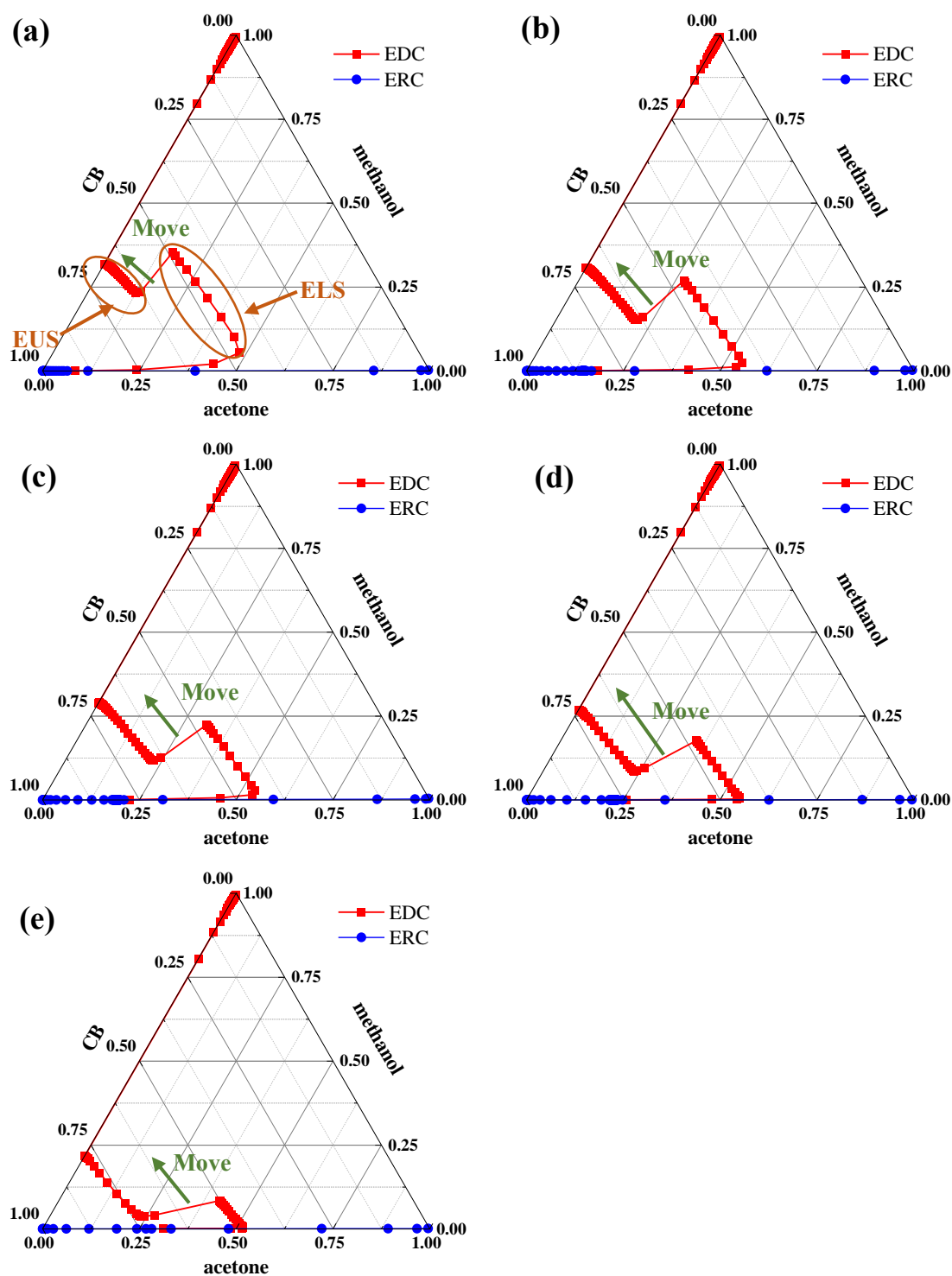trace Acetone
0.0001 Methanol
0.9999 water

Figure S3 Optimization results of extractive distillation schemes using water as the entrainer with stream information for separating acetone-methanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

Figure S4 Optimization results of extractive distillation schemes using CB as the entrainer with stream information for separating acetone-methanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

Figure S5 Composition distribution within the column of extractive distillation schemes using furfural as the entrainer for separating ethyl acetate-ethanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

Figure S6 Composition distribution within the column of extractive distillation schemes using CB as the entrainer for separating acetone-methanol, and the feed composition is (a) 0.2-0.8, (b) 0.4-0.6, (c) 0.5-0.5, (d) 0.6-0.4, and (e) 0.8-0.2.

Table S1. The formulas and parameters used for economic optimization. (Hu et al., 2023)

Parameters	Formula or data	Units
Condenser:		
Heat transfer coefficient (U_C)	0.852	$kW/(K \cdot m^2)$
Temperature difference (ΔT)	T_C-T_0 (298.15 K)	K
Heat transfer area (A_C)	$Q_C/(U_C \times \Delta T)$	m^2
Investment costs	$(M\&S/280) \times 1609.13 \times A_C^{0.65}$	$
Reboiler:		
Heat transfer coefficient (U_R)	0.568	$kW/(K \cdot m^2)$
Temperature difference (ΔT)	T_{LP} (433.15 K)-T_R	K
Heat transfer area (A_R)	$Q_R/(U_R \times \Delta T)$	m^2
Investment costs	$(M\&S/280) \times 1775.26 \times A_R^{0.65}$	$
Column vessel:		
h_{col}	$1.2 \times 0.6096 \times (N_T\text{-}2)$	m
h_{tray}	$0.6096 \times (N_T\text{-}2)$	m
TC_{inst}	$(M\&S/280) \times 97.243 \times D^{1.55} \times h_{tray}$	$
CSC_{inst}	$(M\&S/280) \times 3919.32 \times D^{1.066} \times h_{col}^{0.802}$	$
Investment costs	$TC_{inst} + CSC_{inst}$	$
Energy cost (LP steam)	7.78×10^{-6}	$/kJ
M&S	1582.3 (2016)	–
Payback period	3	year
TAC	(Total equipment cost /Operating period) + operating cost	$/year

References

Hu, N., Zhang, Y., Hu, X., Gu, J., Xue, J., Li, Q., 2023. Efficient Single-Column Extractive Distillation Process Achieved through Vapor–Liquid Separation of Feed. Ind. Eng. Chem. Res. https://doi.org/10.1021/acs.iecr.3c02951

Table S2. Results of correlation with three thermodynamic models for separating ethyl acetate-ethanol.

system	Root mean square deviations		
	UNIQUAC	NRTL	Wilson
Ethanol-Ethyl acetate	0.0131	0.0135	0.0947
Ethanol-EG	0.0334	0.0397	0.0357
Ethanol-Furfural	0.0411	0.0429	0.0416
Ethyl acetate-Furfural	0.0027	0.0045	0.0091
Ethanol-PG	0.0081	0.0078	0.0079
Ethanol-p-Xylene	0.0196	0.0203	0.0157

Table S3. Energy consumption of extractive distillation process under different feed compositions for separating ethyl acetate-ethanol: (a) EG and (b) furfural.

Feed composition (Ethyl acetate-ethanol)	Energy consumption/ kW					
	Positive entrainer (EG)			Reverse entrainer (Furfural)		
	EDC	ERC	EDC+ERC	EDC	ERC	EDC+ERC
0.2-0.8	1518.37	1816.66	3335.03	3551.65	844.48	4396.13
0.4-0.6	1924.86	1754.55	3679.41	2927.01	1124.44	4051.45
0.5-0.5	2141.25	1734.6	3875.85	2655.93	1267.5	3923.43
0.6-0.4	2479.58	1661.14	4140.72	2405.86	1312.07	3717.93
0.8-0.2	3245.88	1045.51	4291.39	1885.62	1306.85	3192.47

Table S4. Energy consumption of extractive distillation process under different feed compositions for separating acetone-methanol: (a) water and (b) CB.

Feed composition (Acetone-methanol)	Energy consumption/ kW					
	Positive entrainer (Water)			Reverse entrainer (CB)		
	EDC	ERC	EDC+ERC	EDC	ERC	EDC+ ERC
0.2-0.8	1036.9	1593.18	2630.08	2802.77	600.487	3403.257
0.4-0.6	1396.43	1289.84	2686.27	2136.29	694.016	2830.306
0.5-0.5	1641.94	1125.23	2767.17	1864.95	789.9	2654.85
0.6-0.4	1938.19	985.304	2923.494	1643.69	889.718	2533.408
0.8-0.2	2556.21	733.311	3289.521	1196.29	1046.72	2243.01