Electronic Supplementary Material

Optimization and simultaneous heat integration design of a coal-based ethylene glycol refining process by a parallel differential evolution algorithm

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$$C_{cs}(US\$) = 17{,}640D^{1.066}H^{0.802} \tag{S1}$$

$$C_{ct}(US\$) = 229D^{1.55}(NT-2) \tag{S2}$$

$$H\ (m) = 1.2 \cdot 0.61(NT-2) \tag{S3}$$

$$C_{hex}(US\$) = 7{,}296A^{0.65} \tag{S4}$$

$$A\ (m^2) = \frac{Q}{U \cdot LMTD} \tag{S5}$$

Table S1. The parameters of coupling reaction kinetic

	Pre exponential factor	Activation energy
Kinetic parameters		
K_a	1.46×10^{9}	6.895×10^{4}
K_b	4.1×10^{12}	3.945×10^{4}
K_c	1.89×10^{5}	6.312×10^{4}

Table S2. The parameters of hydrogenation reactions kinetic

	Pre exponential factor	Activation energy
Kinetic parameters		
k_1	3.87×10^{7}	44,284
k_2	1.75×10^{6}	37,710
k_3	8.78×10^{13}	137,380
Equilibrium constant		
K_{Me}	5.49×10^{-12}	66,356
K_{EG}	1.85×10^{-4}	18,883
K_{MG}	2.65×10^{-2}	19,242
K_{DMO}	7.92×10^{-5}	118,170
K_{H2}	1.20×10^{3}	8,348
K_{p1}	163.4161	17,759
K_{p2}	0.2873	15,921

Table S3. The parameters of oxidation and dehydration reaction kinetic

Reaction rate constant			
k_1	45×10^6	E_1	79,500
k_2	40,320	E_2	66,900
k_3	24,953	E_3	62,800
Equilibrium constant			
K_a	27	E_a	8,368

Table S4. The types and prices of utilities

	Utility	Price/US$/GJ
	low-pressure steam (LPS, 6bar/160°C)	7.78
C_{hu}	medium-pressure steam (MPS, 11bar/184°C)	8.22
	high-pressure steam (HPS, 42bar, 254°C)	9.88
C_{cu}	cooling water (30°C-40°C)/ (5°C -15°C)	0.354/ 4.43
C_{ref}	refrigerant (-20°C)	7.89

Table S5. Variable range of each column

Column	Column parameters				
	Rectifying stages	Stripping stages	Reflux ratio	Top pressure /kPa	Recycle stage
C1	3-75	3-75	0.01-15	50-700	/
C2	3-75	3-75	0.01-15	50-700	/
C3	3-60	3-30	1-15	50-3000	3-60
C4	3-75	3-75	0.01-15	50-700	/
C5	3-75	3-75	0.01-15	50-700	/
C6	3-75	3-75	0.01-15	25-700	/
C7	3-75	3-75	0.01-15	50-700	/
C8	3-75	3-75	0.01-15	50-700	/

Table S6. Enthalpy and latent heat of steam

Steam	Enthalpy/kJ/kg	Latent heat/kJ/kg
LPS	2680.2	2081.7
MPS	2715.9	1998.6
HPS	2790.3	1692.6

Table S7. Binary interaction parameters from aspen built-in

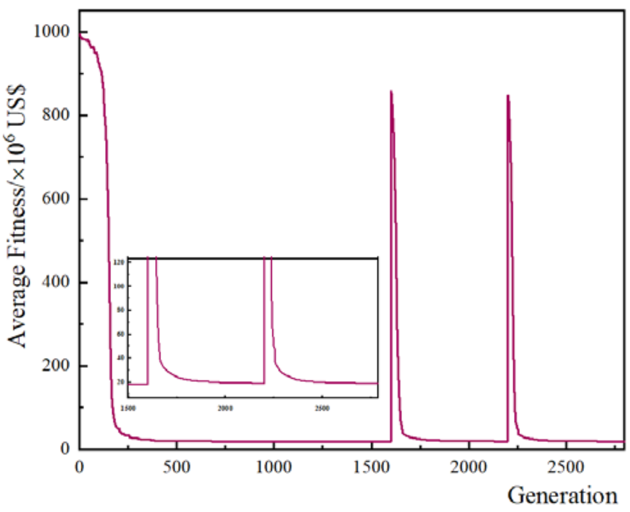
Component i	Component j	A_{IJ}	A_{JI}	B_{IJ}	B_{JI}	C_{IJ}	D_{IJ}	E_{IJ}	E_{JI}	F_{IJ}	F_{JI}
NH_3	H_2O	9.6121	-6.2684	-3232.82	1525.454	0.3	0	0	0	0	0
H_2O	CH_4O	2.7322	-0.693	-617.269	172.9871	0.3	0	0	0	0	0
H_2O	DMO	-456.474	-232.384	22864.88	12859.65	0.2	0	67.0785	33.6488	0	0
H_2O	EG	0.3479	-0.0567	34.8234	-147.137	0.3	0	0	0	0	0
CH_4O	EG	33.3298	0.1753	-10000	-322.924	0.3	0	0	0	0	0
H_2O	ET	3.4578	-0.8009	-586.081	246.18	0.3	0	0	0	0	0
CH_4O	ET	4.7119	-2.3127	-1162.29	483.8436	0.3	0	0	0	0	0
EG	ET	-0.1115	14.8422	157.5937	-4664.41	0.47	0	0	0	0	0

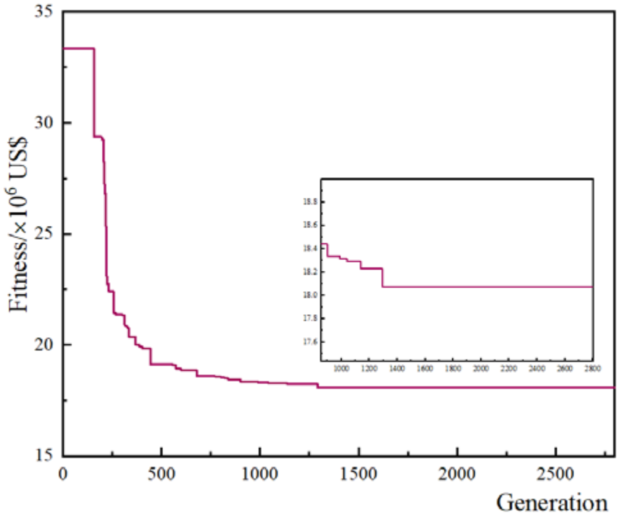
Table S8. Stream composition

Composition	C1				C2			C3			C4		C5			C6		C7		C8	
Mol/%	F	T_G	T_L	B	F	T	B	F	T	B	T	B	F	T	B	T	B	T	B	T	B
CO	0	2.01	0	0	0	0	0	4.04	5.24	0	0	0	0	3.88	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0	0	0	0	0	0	0	2.89	0	0	0	0	0	0	0
H2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0	0	0	0	0	0	0	0.40	0	0	0	0	0	0	0
H2S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
COS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NH3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2O	0	0	0	0	0	0	0	0	0	91.57	67.72	98.72	4.45	0.16	4.46	0	11.58	20.38	9.83	49.58	0
CH4O	96.35	41.45	97.28	0.21	97.28	98.72	0.80	4.91	0.14	7.05	26.57	1.19	61.37	24.44	61.44	98.68	1.89	10.36	0.21	1.05	0
O2	0	0	0	0	0	0	0	18.14	0.09	0	0	0	0	0	0	0	0	0	0	0	0
MN	0.42	1.81	0.41	0	0.41	0.42	0	0.58	94.53	1.34	5.68	0.04	0.09	49.23	0	0	0	0	0	0	0
DMO	0.38	0	0	99.43	0	0	0.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NO	0.58	54.34	0.04	0	0.04	0.04	0	72.31	0	0	0	0	0.03	18.1	0	0	0	0	0	0	0
EG	0	0	0	0	0	0	0	0	0	0	0	0	26.16	0	26.21	0	68.11	0.14	81.64	7.62	99.93
DMC	2.24	0.40	2.26	0.36	2.26	0.82	99.08	0.02	0	0.04	0.03	0.05	3.35	0.29	3.36	0.02	8.69	12.86	7.86	39.66	0
MG	0	0	0	0	0	0	0	0	0	0	0	0	0.08	0	0.08	0	0.21	0.03	0.24	0.95	0.07
ET	0	0	0	0	0	0	0	0	0	0	0	0	4.44	0.59	4.46	1.29	9.5	56.23	0.22	1.11	0

※T_G and T_L represent the gas and liquid outlet of column top, respectively

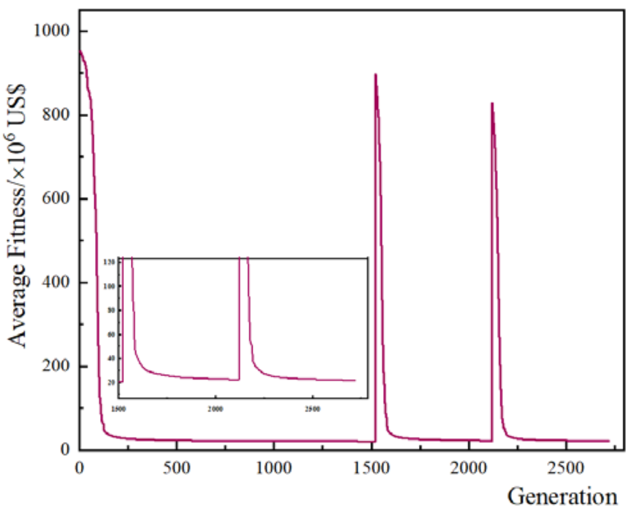
※The feed stream of C4, C6, C7 and C8 is the bottom outlet of C3, C5, C6 and C7, respectively

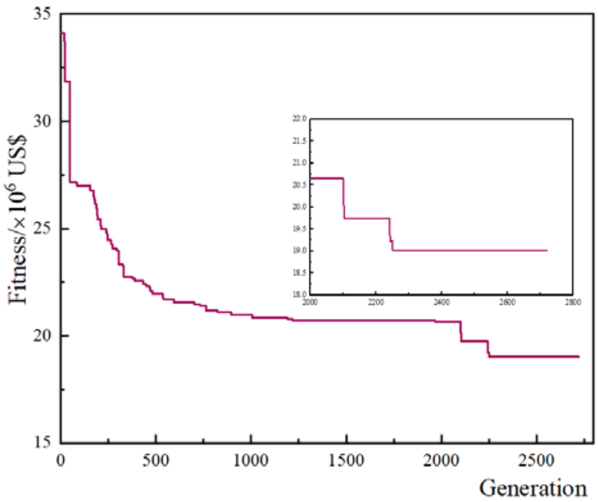




(a) Fitness average curve (SI)

(b) Fitness curve (SI)

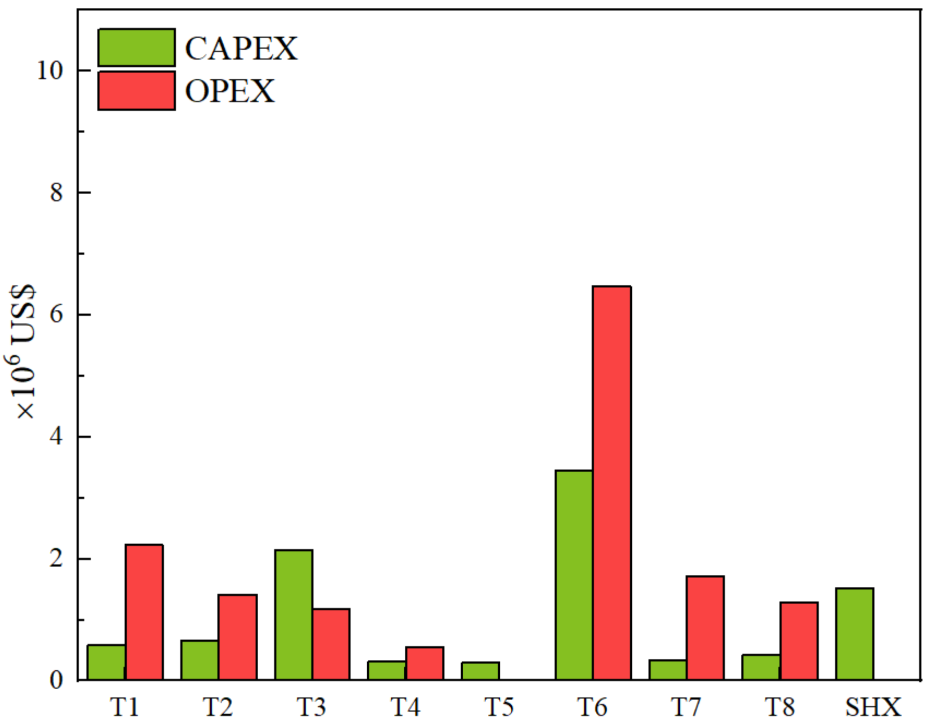




(c) Fitness average curve (SE)

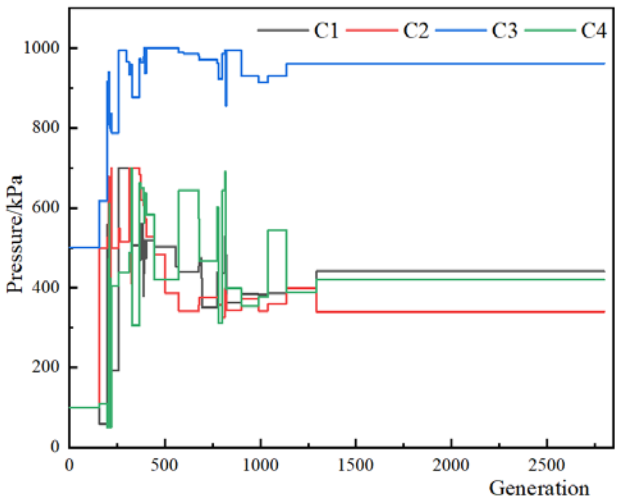
(d) Fitness curve (SE)

Fig. S1. Evolution curve

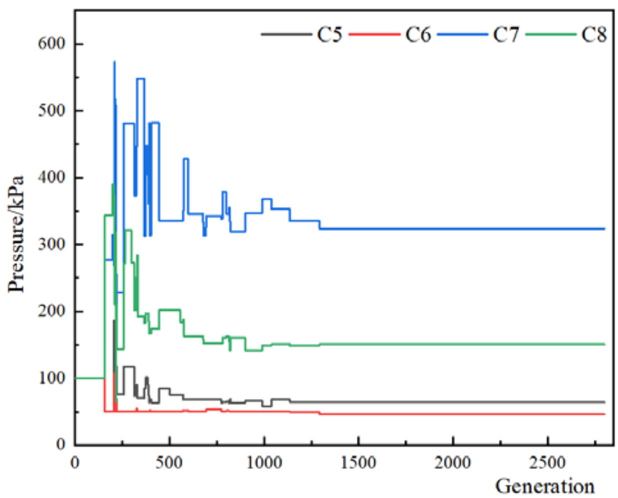


※SHX represents the streams heat exchangers

Fig. S2. The annual CAPEX and OPEX of each column in the SI-Optimized configuration

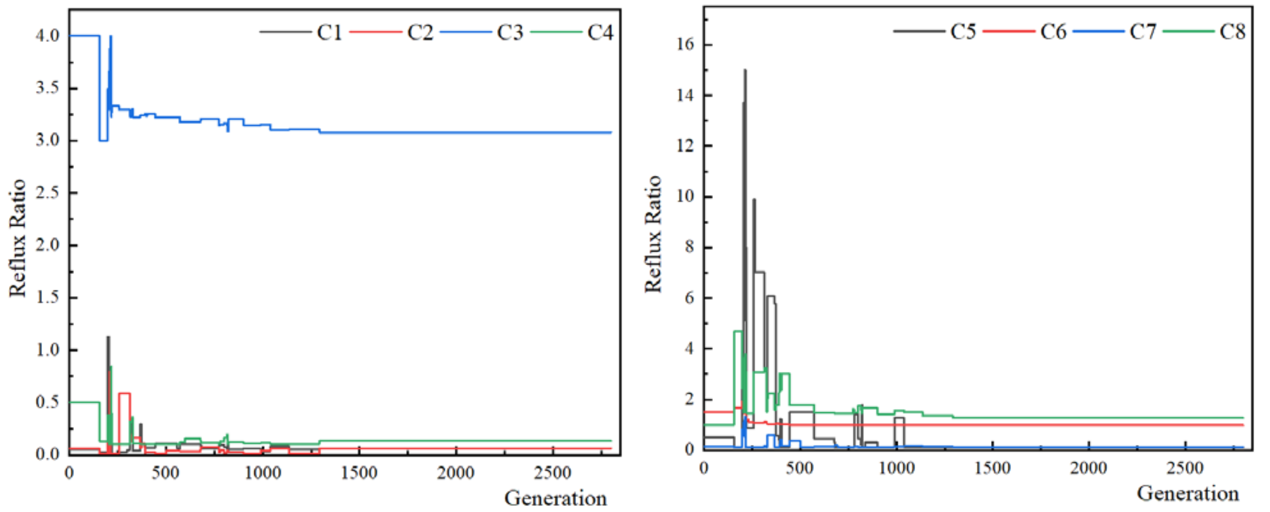


(a) C1-C4



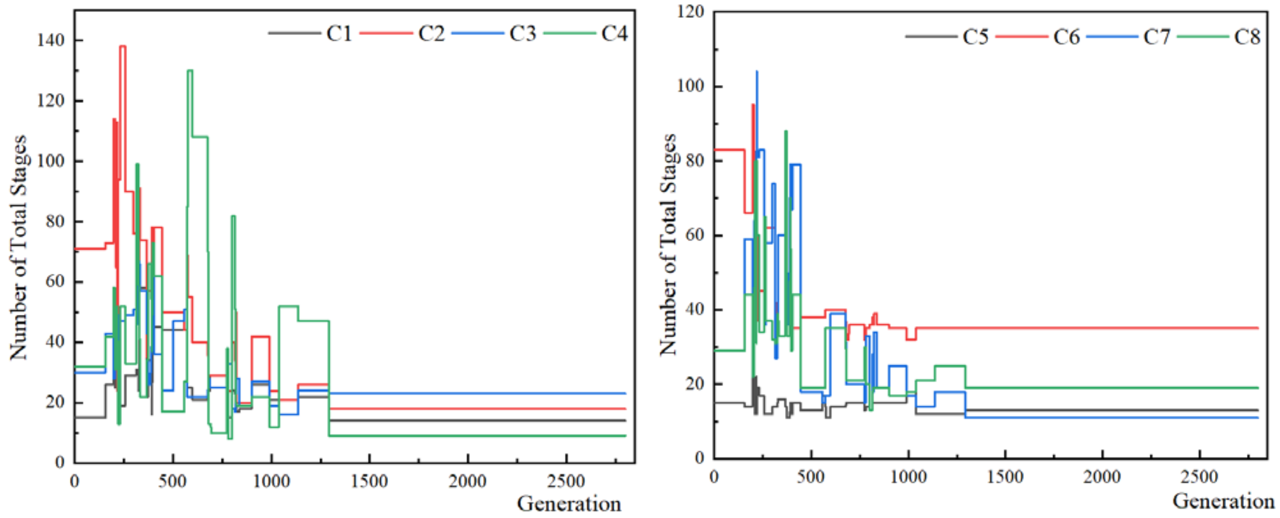
(b) C5-C8

Fig. S3. Operating pressure evolution curve



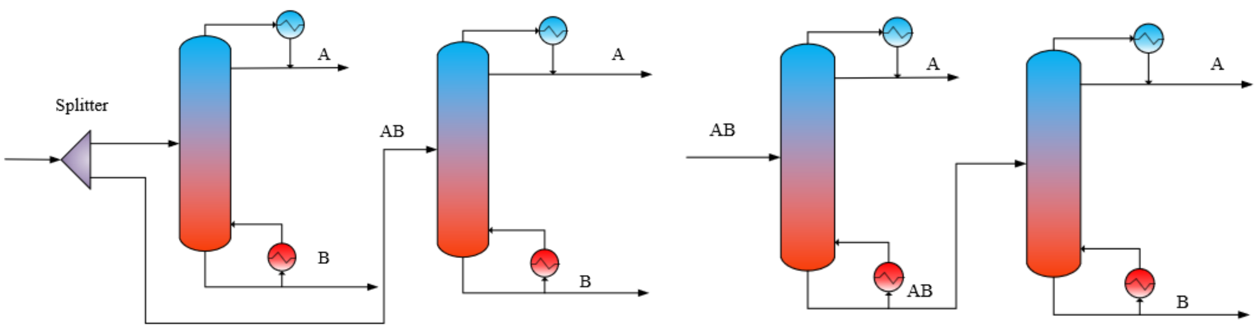
(a) C1-C4 **(b) C5-C8**

Fig. S4. Reflux ratio evolution curve

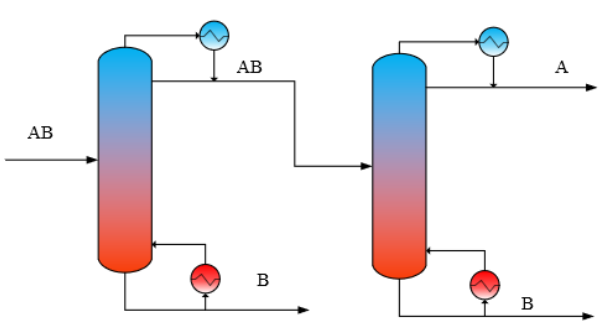


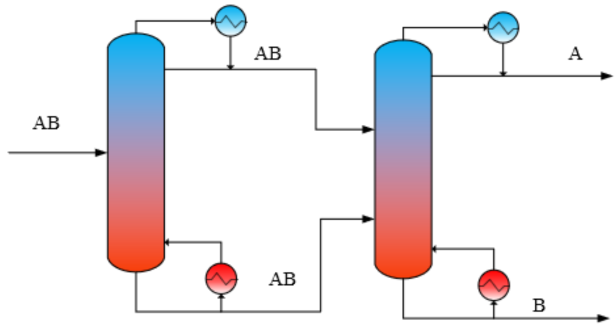
(a) C1-C4 **(b) C5-C8**

Fig. S5. Number of total stages evolution curve

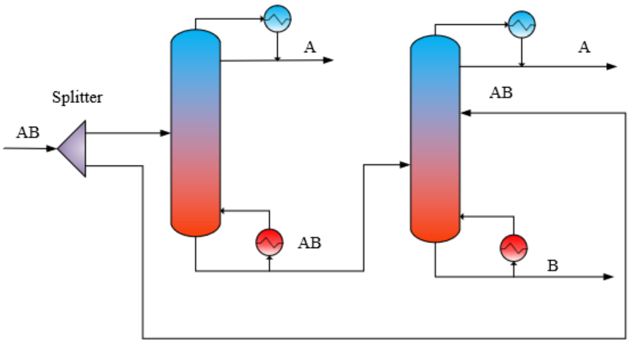


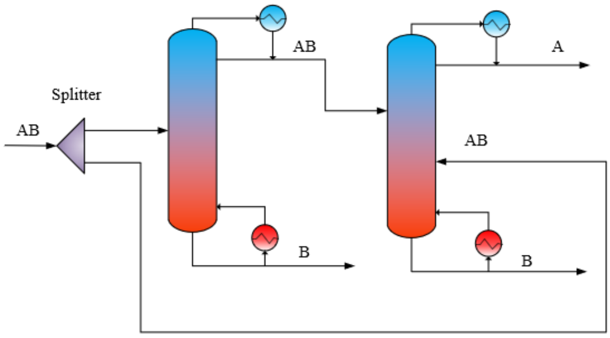
(a) Feed split **(b) Lights split**



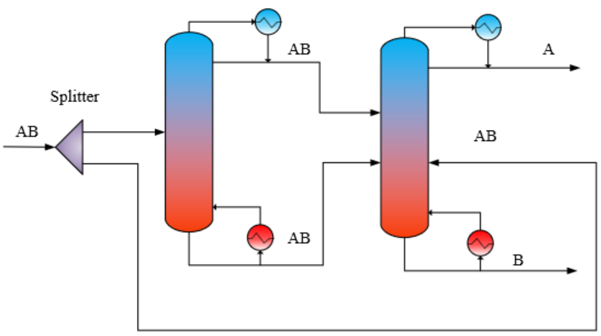


(c) Heavies split **(d) Pre-fraction splits**





(e) Feed split and Lights split **(f) Feed split and Heavies split**



(g) Feed split and Pre-fraction split

Fig. S6. 7 different double-effect configurations

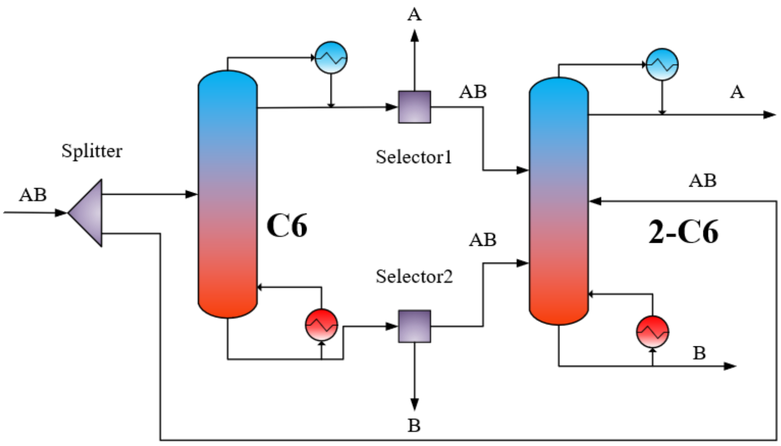
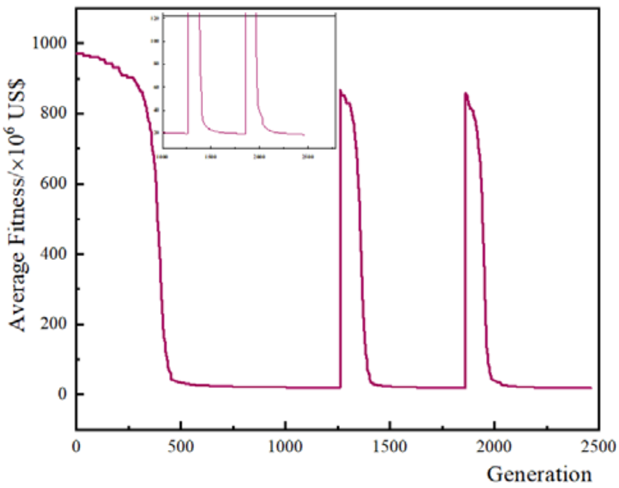
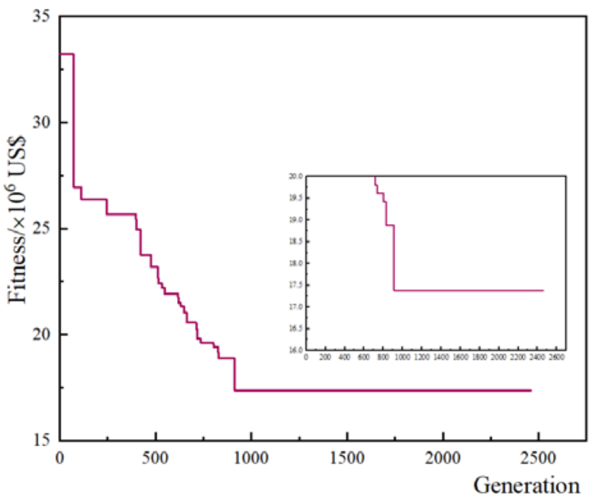
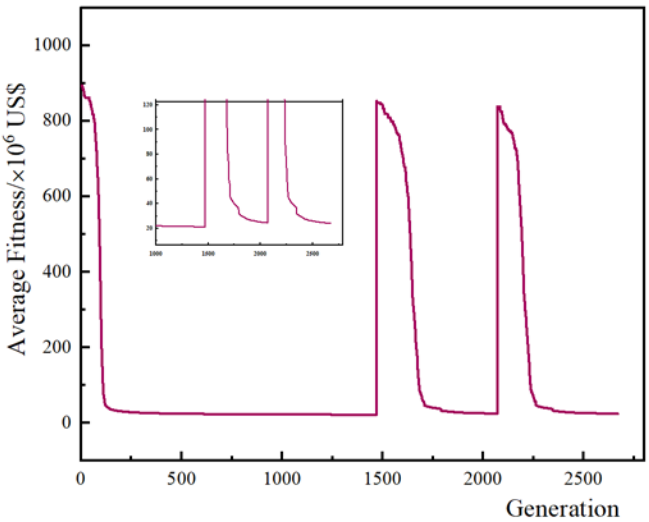


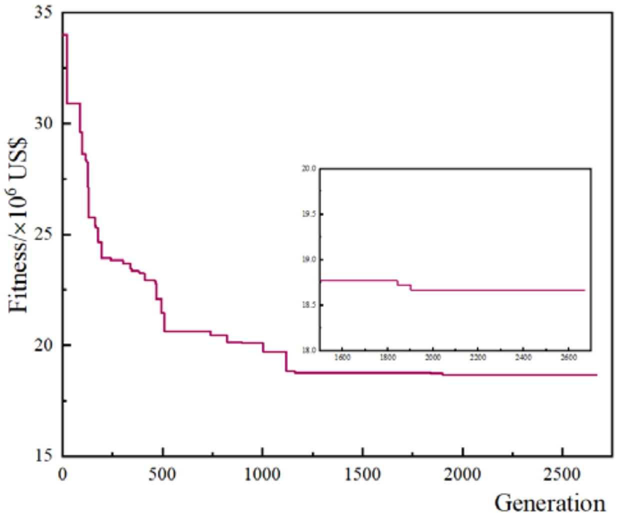
Fig. S7. C6 Superstructure





(a) Fitness average curve (SI) **(b) Fitness curve (SI)**





(c) Fitness average curve (SE) **(d) Fitness curve (SE)**

Fig. S8. Evolution curve of superstructure optimization

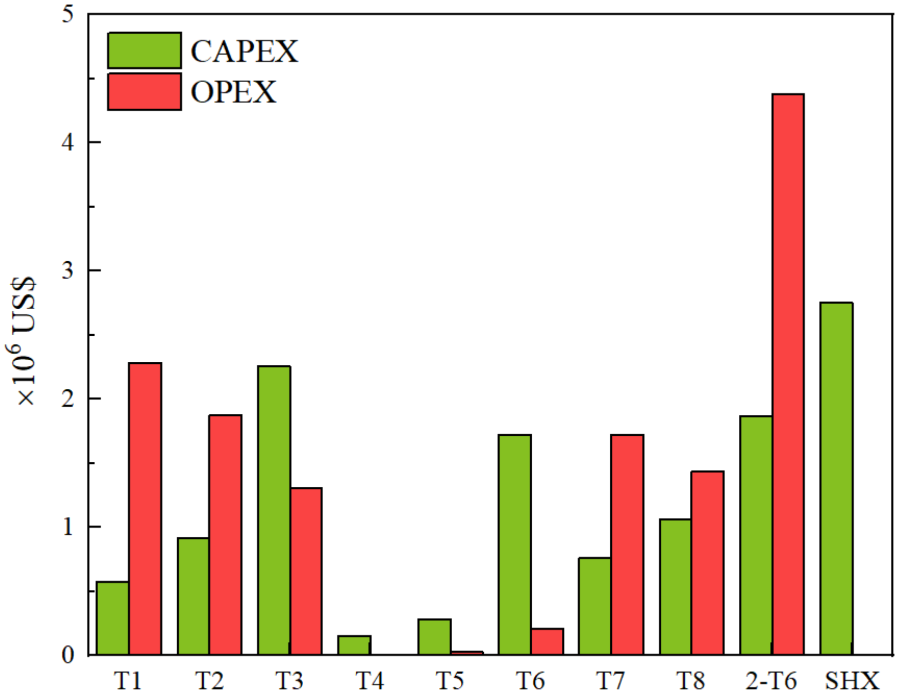
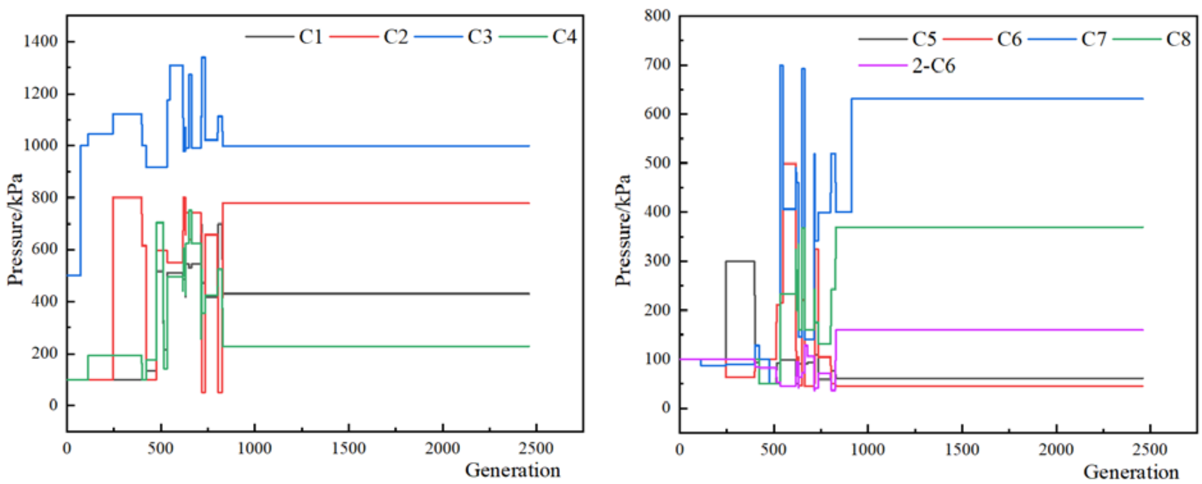
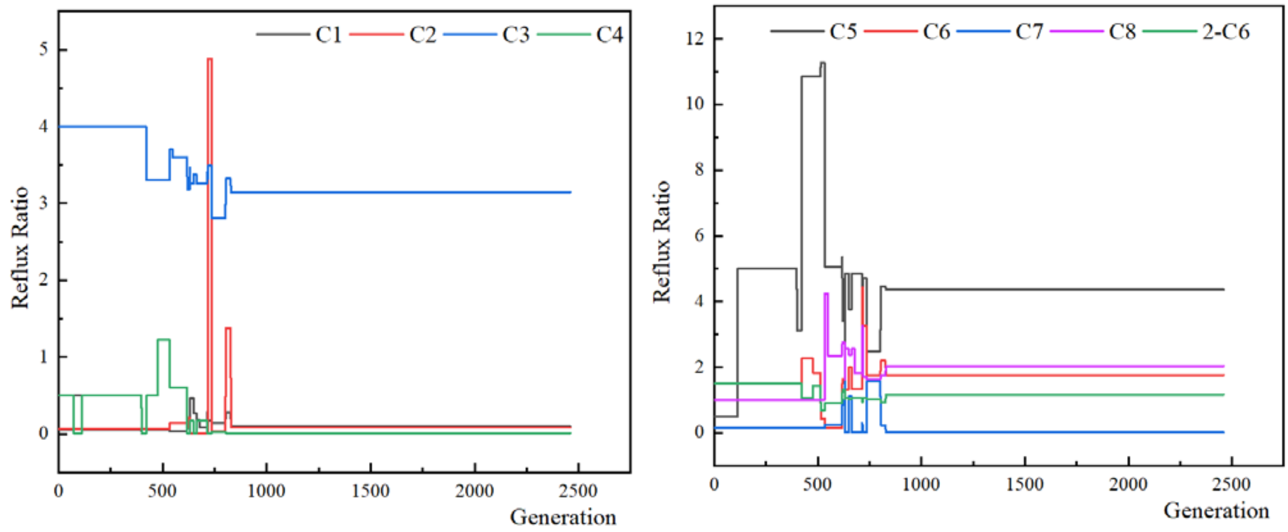


Fig. S9. The annual CAPEX and OPEX of each column in the SI-Superstructure configuration



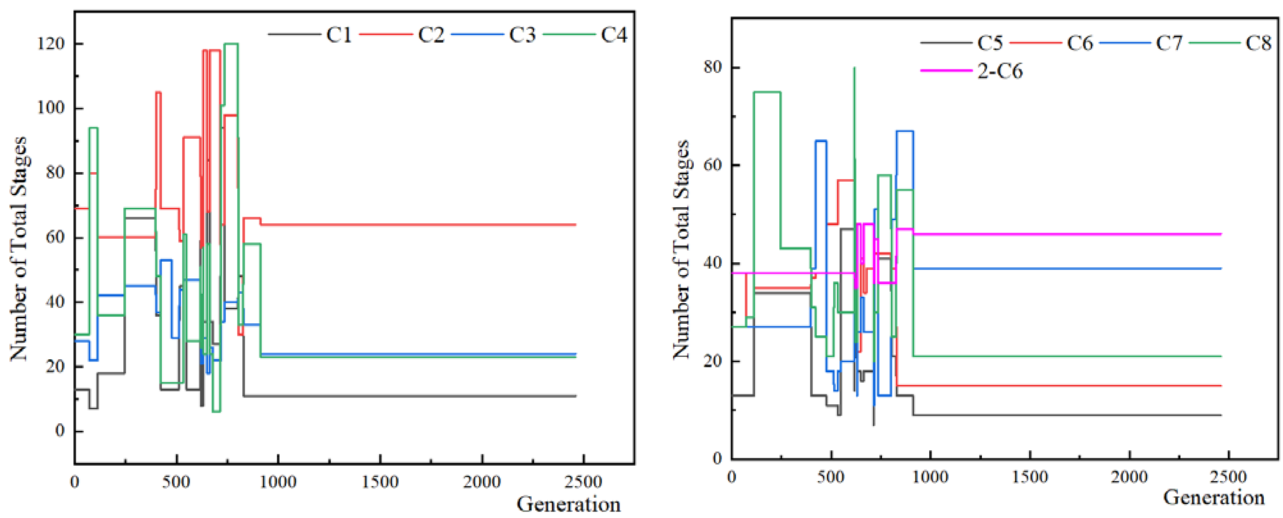
(a) C1-C4 **(b) C5-2-C6**

Fig. S10. Operating pressure evolution curve



(a) C1-C4 **(b) C5-2-C6**

Fig. S11. Reflux ratio evolution curve



(a) C1-C4 **(b) C5-2-C6**

Fig. S12. Number of total stages evolution curve