Supporting Information

Energy-efficient design of downstream separation to produce n-butanol by several heat integrated technologies

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Table S1 Basis of economics

Condensers costs

Heat-transfer coefficient=0.852kW/(K·m^2)

Capital cost=$7296Ac^{0.65}$, where area is in squared meters

Reboilers costs

Heat-transfer coefficient=0.568kW/(K·m^2)

Capital cost=$7296A_R^{0.65}$, where area is in squared meters

Coolers costs

Overall heat-transfer coefficient of the systems with liquid phases on both sides is 0.57 kW/K•m^2

Capital cost=$7296A_R^{0.65}$, where area is in squared meters

Column vessel costs

Capital cost=$17640\ D^{1.066}\ L^{0.802}$

Where D is using aspen tray sizing while $L=(N_T-1)\times0.61+6$

Compressor costs

Capital cost=$1293/280\times1264.75\times(hp)^{0.82}$

Where hp represents the horse power of compressor

Annual steam cost

Steam cost=Cs×Q×8000×3600

Where Cs=$7.72 per GJ /LP steam (433K)

Cs=$8.22 per GJ /MP steam (457K)

Annual cooling water cost

Cooling water cost=$0.03\times Q_c/(\Delta T_W\times4.183\times1000)\times8000\times3600$

Electricity costs

Electricity cost=16.8×hp/0.72×8000×3.6/1000

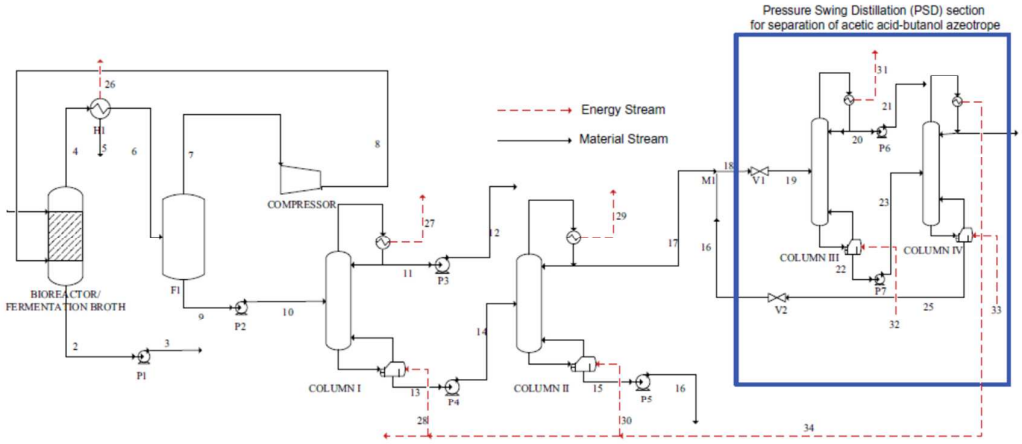

Fig. 2. Fermentation broth separation using gas stripping and distillation process.

it can be calculated based on the material balance of the COLUMN I, COLUMN II, COLUMN III and COLUMN IV.

$$F_{S10}=F_{S12}+F_{S16}+F_{S21}+F_{S24}$$

Table S2. Stream results of stream 10

Stream No	Butanol	Acetone	Ethanol	Acetic acid	Butyric acid	water	Total mass flowrate (kg/h)
Option B							
12	0.0000	0.0024	0.0005	0.0000	0.0000	0.0002	0.0031
16	0.0000	0.0000	0.0000	0.0000	0.0062	0.0000	0.0062
21	0.0001	0.0000	0.0000	0.0054	0.0000	0.0000	0.0055
24	0.0048	0.0000	0.0000	0.0000	0.0000	0.0000	0.0048
10	0.0049	0.0024	0.0005	0.0054	0.0062	0.0002	0.0196

Table S2A. Energy consumption of reboilers of Column I, Column II, Column III and Column IV in the literature

Process simulation results	Process specific results
	Option B
Energy consumption rate (kW)	
Reboilers	
Column I	0.0039
Column II	0.0025
Column III	0.561
Column IV	0.7954
Total	1.3628

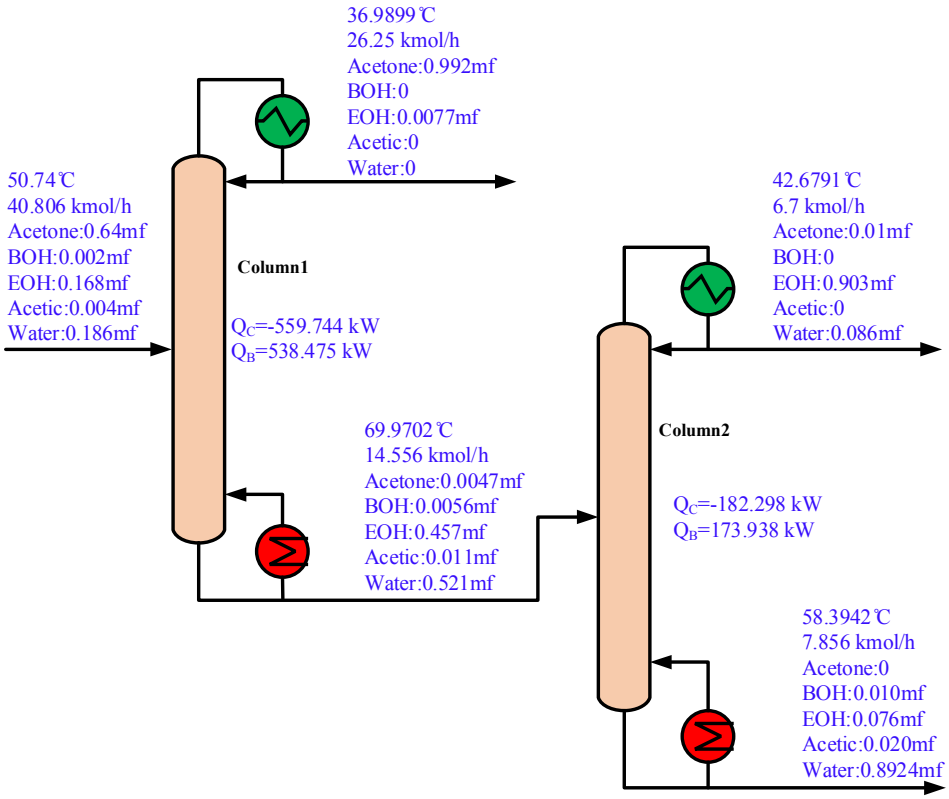

Fig S1. Flowsheet of separation of acetone and ethanol

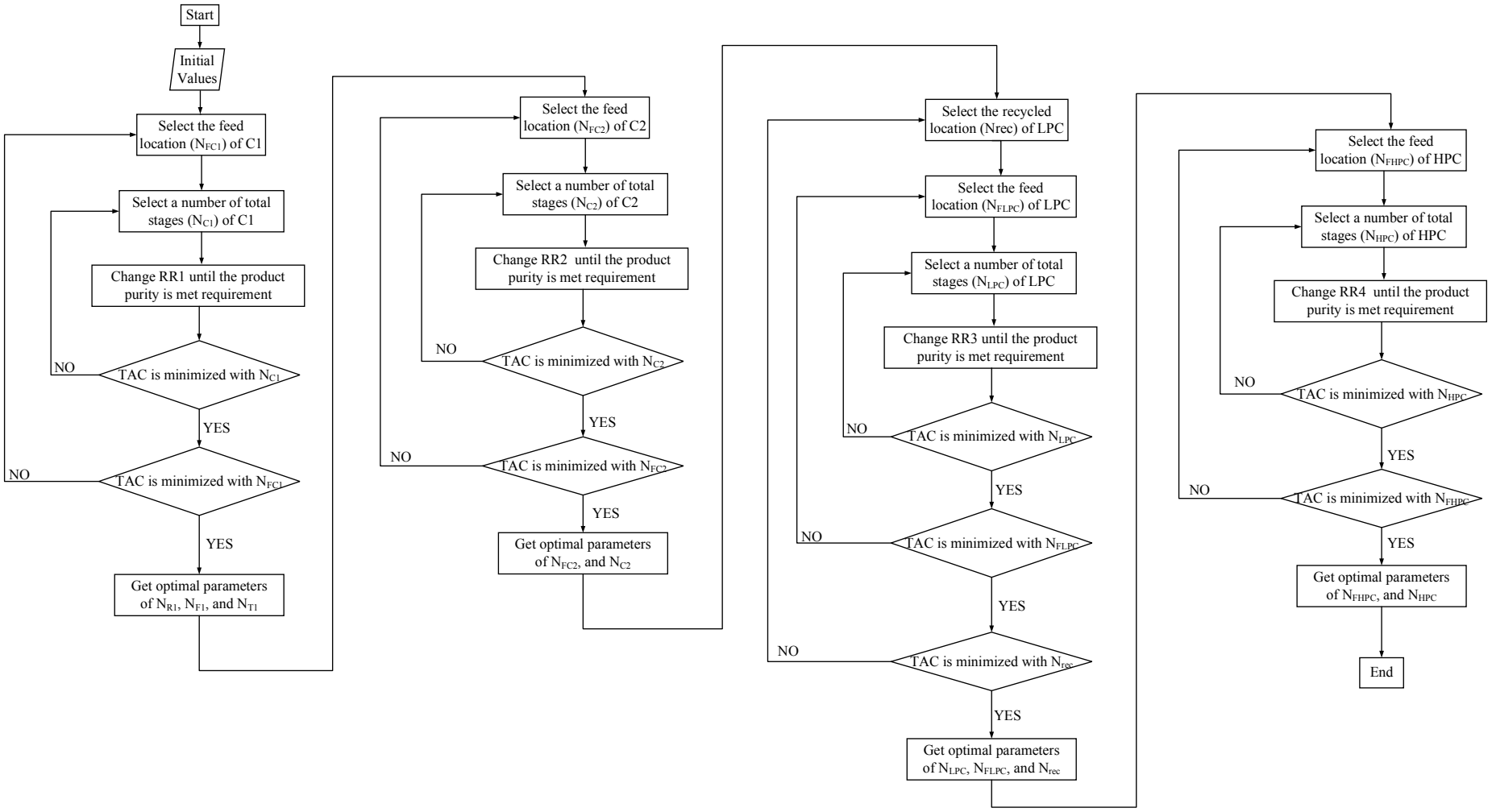

Fig S2. Sequential iterative optimization procedure of the base process

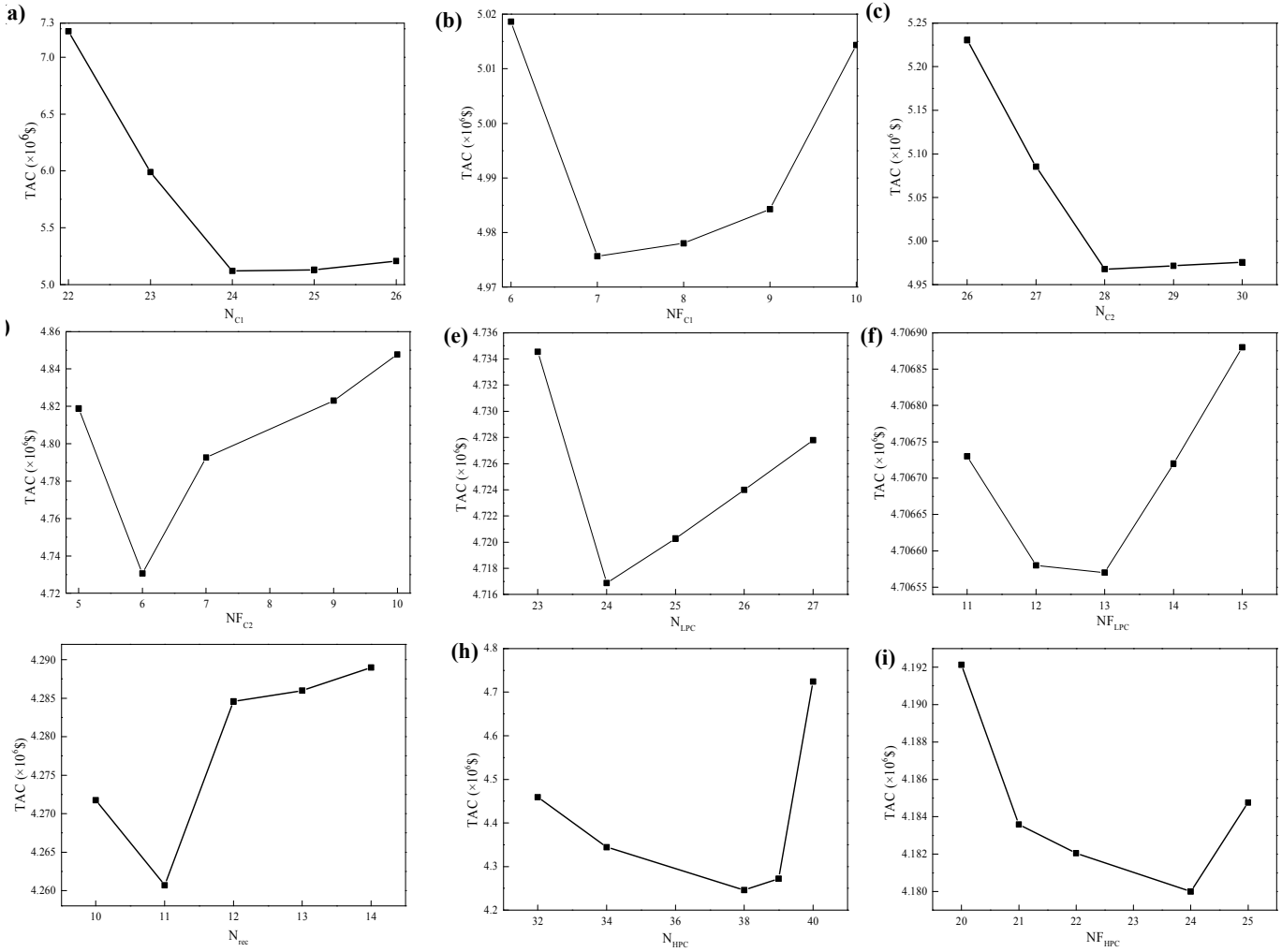

Fig S3. Optimal results of the base process

Table S3. Basic parameters of the Base process

Item		Base process			
Distillation Columns					
		C1	C2	LPC	HPC
Reflux Ratio		5.2	0.75	7.9	14
Diameter (m)		1.454	1.949	2.763	1.794
Total Stage（N_T)		24	28	24	38
Feed Tray (N_F)		12	14	13	24
Recycled Feed tray (N_r)		/	/	11	/
Condensers					
	Heat duty (kW)			2481.69	
C1-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			168.39	
	Heat duty (kW)			1804.51	
C2-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			69.92	
	Heat duty (kW)			3422.97	
LPC-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			176.14	
	Heat duty (kW)			6578.76	
HPC-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			60.40	
Reboilers					
	Heat duty (kW)			2489.88	
C1-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			96.59	
	Heat duty (kW)			1502.18	
C2-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			43.96	
	Heat duty (kW)			3391.46	
LPC-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			63.15	
	Heat duty (kW)			6592.12	
HPC-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			712.90	

Table S3. Basic parameters of the Base process (Continued)

Item		Base process	
Heaters			
	H1	Heat duty (kW)	560.41
		Overall heat-transfer coefficients (kW/K·m^2)	0.568
		Heat-transfer areas (m^2)	11.59
	H2	Heat duty (kW)	417.96
		Overall heat-transfer coefficients (kW/K·m^2)	0.568
		Heat-transfer areas (m^2)	121.42
Coolers			
	Coolers1	Heat duty (kW)	25.90
		Overall heat-transfer coefficients (kW/K·m^2)	0.57
		Heat-transfer areas (m^2)	4.05
	Coolers2	Heat duty (kW)	130.93
		Overall heat-transfer coefficients (kW/K·m$_2$)	0.57
		Heat-transfer areas (m^2)	6.96
	Coolers3	Heat duty (kW)	58.33
		Overall heat-transfer coefficients (kW/K·m^2)	0.57
		Heat-transfer areas (m^2)	7.22
	Coolers4	Heat duty (kW)	263.14
		Overall heat-transfer coefficients (kW/K·m^2)	0.57
		Heat-transfer areas (m^2)	11.78
	Coolers5	Heat duty (kW)	154.05
		Overall heat-transfer coefficients (kW/K·m^2)	0.57
		Heat-transfer areas (m^2)	2.26

Table S4. Basic parameters of the HI-A process

Item		HI-A process			
Distillation Columns					
		C1	C2	LPC	HPC
Reflux Ratio		5.2	0.75	7.9	14
Diameter (m)		1.454	1.949	2.763	1.794
Total Stage (N_T)		24	28	24	38
Feed Tray (N_F)		12	14	13	24
Recycled Feed tray (N_r)		/	/	11	/
Condensers					
	Heat duty (kW)			2481.69	
C1-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			168.39	
	Heat duty (kW)			1804.51	
C2-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			69.92	
	Heat duty (kW)			3422.97	
LPC-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			176.14	
	Heat duty (kW)			6578.76	
HPC-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			60.40	
Reboilers					
	Heat duty (kW)			3391.46	
LPC-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			63.15	
	Heat duty (kW)			6592.12	
HPC-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			712.90	
Heaters					
	Heat duty (kW)			263.90	
H2	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			10.09	
Self-Heat Exchangers					
	Heat duty (kW)			560.41	
E1	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			11.59	
	Heat duty (kW)			2489.88	
E2	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			63.15	
	Heat duty (kW)			1502.18	
E3	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			712.90	

Table S4. Basic parameters of the HI-A process (continued)

Item	HI-A process	
	Heat duty (kW)	154.05
E4	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	11.88
Coolers		
	Heat duty (kW)	25.90
Coolers1	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	4.05
	Heat duty (kW)	130.93
Coolers2	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	6.96
	Heat duty (kW)	58.33
Coolers3	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	7.22
	Heat duty (kW)	263.14
Coolers4	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	11.78

Table S5. Basic parameters of the HI-B process

Item		HI-B process			
Distillation Columns					
		C1	C2	LPC	HPC
Reflux Ratio		5.2	0.75	7.9	17.11
Diameter (m)		1.454	1.949	2.763	1.986
Total Stage (N_T)		24	28	24	38
Feed Tray (N_F)		12	14	13	24
Recycled Feed tray (N_r)		/	/	11	/
Condensers					
	Heat duty (kW)			2481.69	
C1-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			168.39	
	Heat duty (kW)			1804.51	
C2-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			69.92	
	Heat duty (kW)			3422.97	
LPC-C	Overall heat-transfer coeffic+ients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			176.14	
	Heat duty (kW)			6578.76	
HPC-C	Overall heat-transfer coefficients (kW/K·m^2)			0.852	
	Heat-transfer areas (m^2)			60.40	
Reboilers					
	Heat duty (kW)			7957.24	
HPC-B	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			860.53	
Heaters					
	Heat duty (kW)			263.90	
H2	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			10.09	
Self-Heat Exchangers					
	Heat duty (kW)			560.41	
E1	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			11.59	
	Heat duty (kW)			2489.88	
E2	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			63.15	
	Heat duty (kW)			1502.18	
E3	Overall heat-transfer coefficients (kW/K·m^2)			0.568	
	Heat-transfer areas (m^2)			712.90	
E4	Heat duty (kW)			3391.46	

	Overall heat-transfer coefficients (kW/K·m^2)	0.568
	Heat-transfer areas (m^2)	63.15

Table S5. Basic parameters of the HI-B process (continued)

Item	HI-B process	
	Heat duty (kW)	154.05
E5	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	11.88
Coolers		
	Heat duty (kW)	25.90
Coolers1	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	4.05
	Heat duty (kW)	130.93
Coolers2	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	6.96
	Heat duty (kW)	58.33
Coolers3	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	7.22
	Heat duty (kW)	263.14
Coolers4	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	11.78

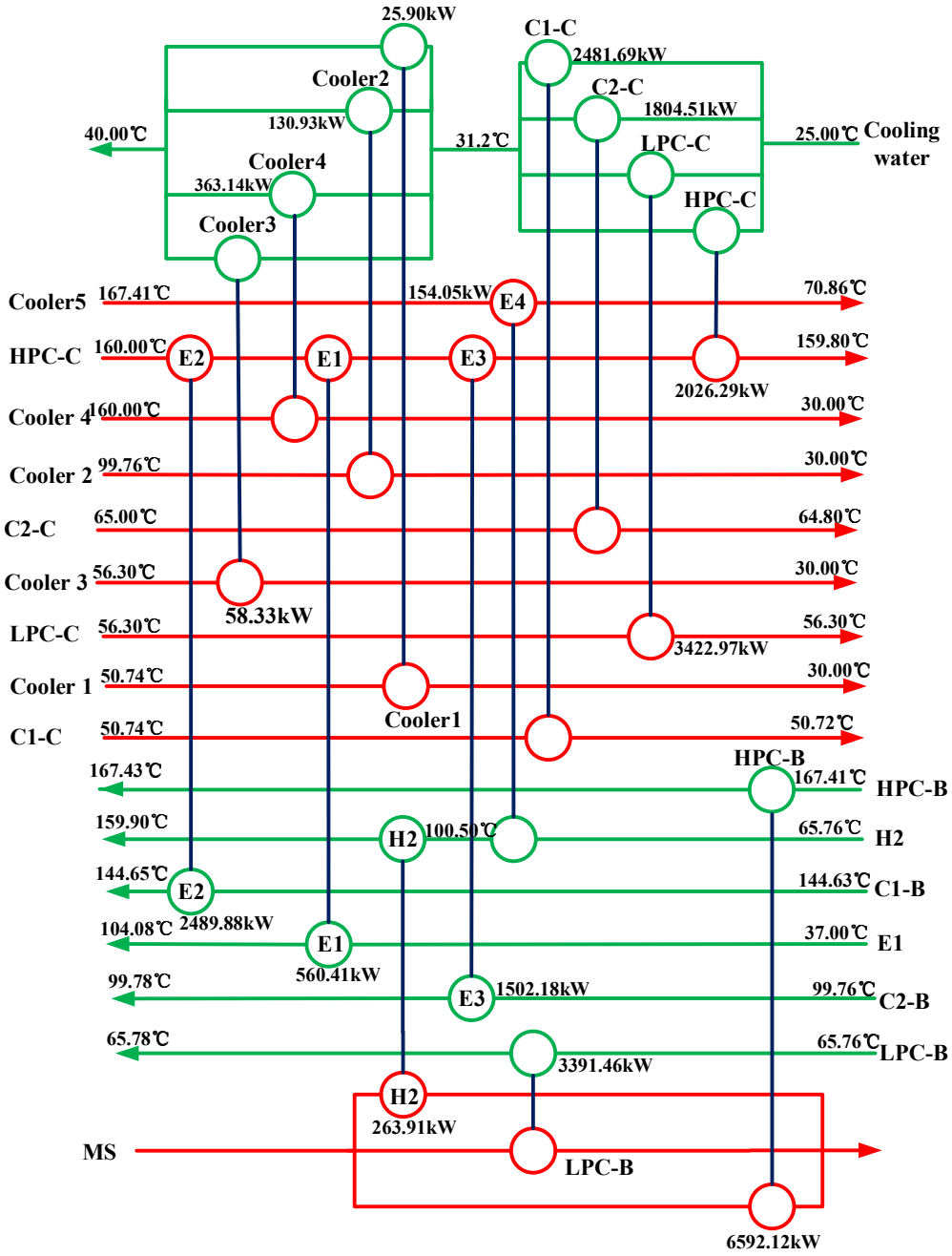

Fig S4. Heat exchanger network (HEN) of the HI-A process

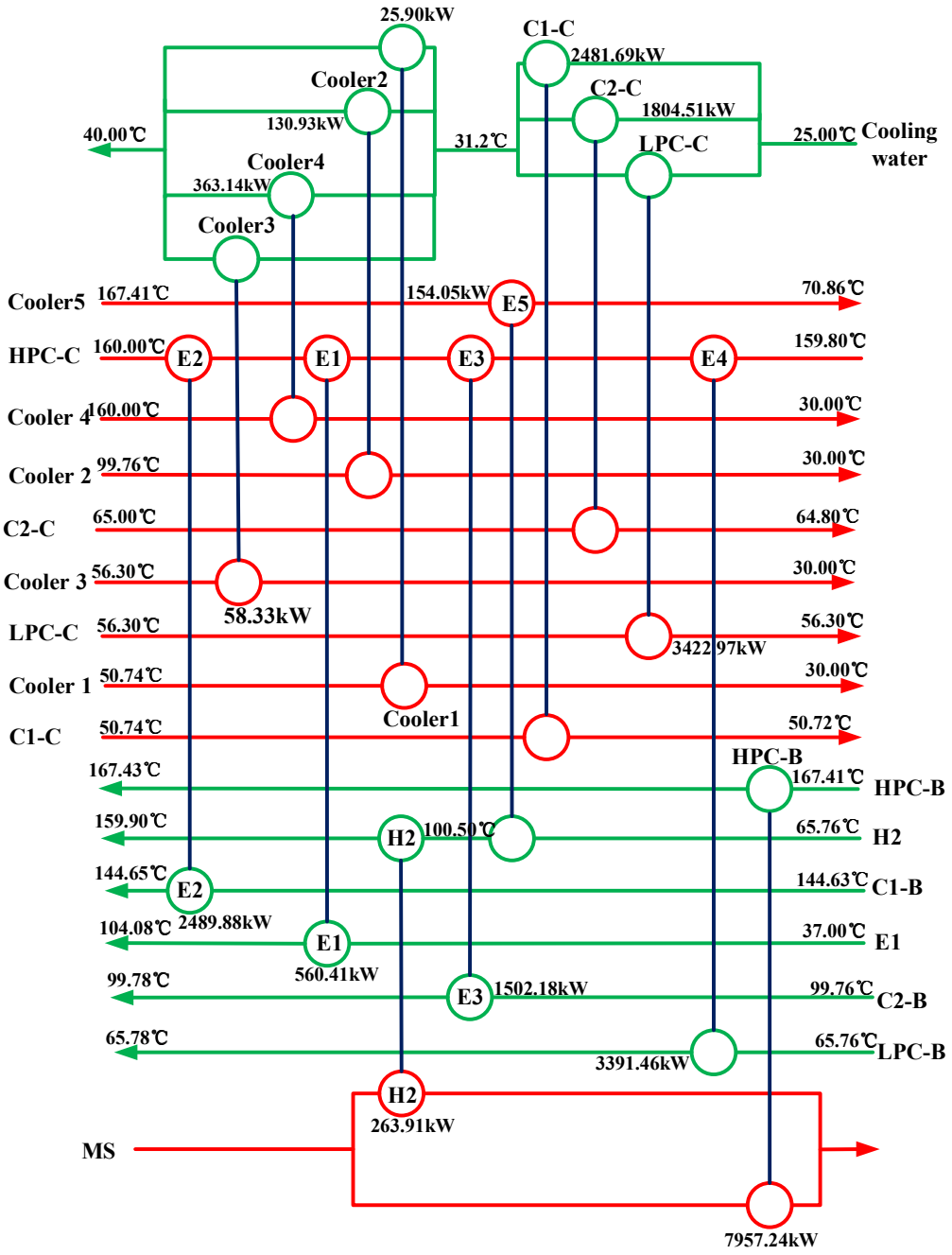

Fig S5. HEN of the HI-B process

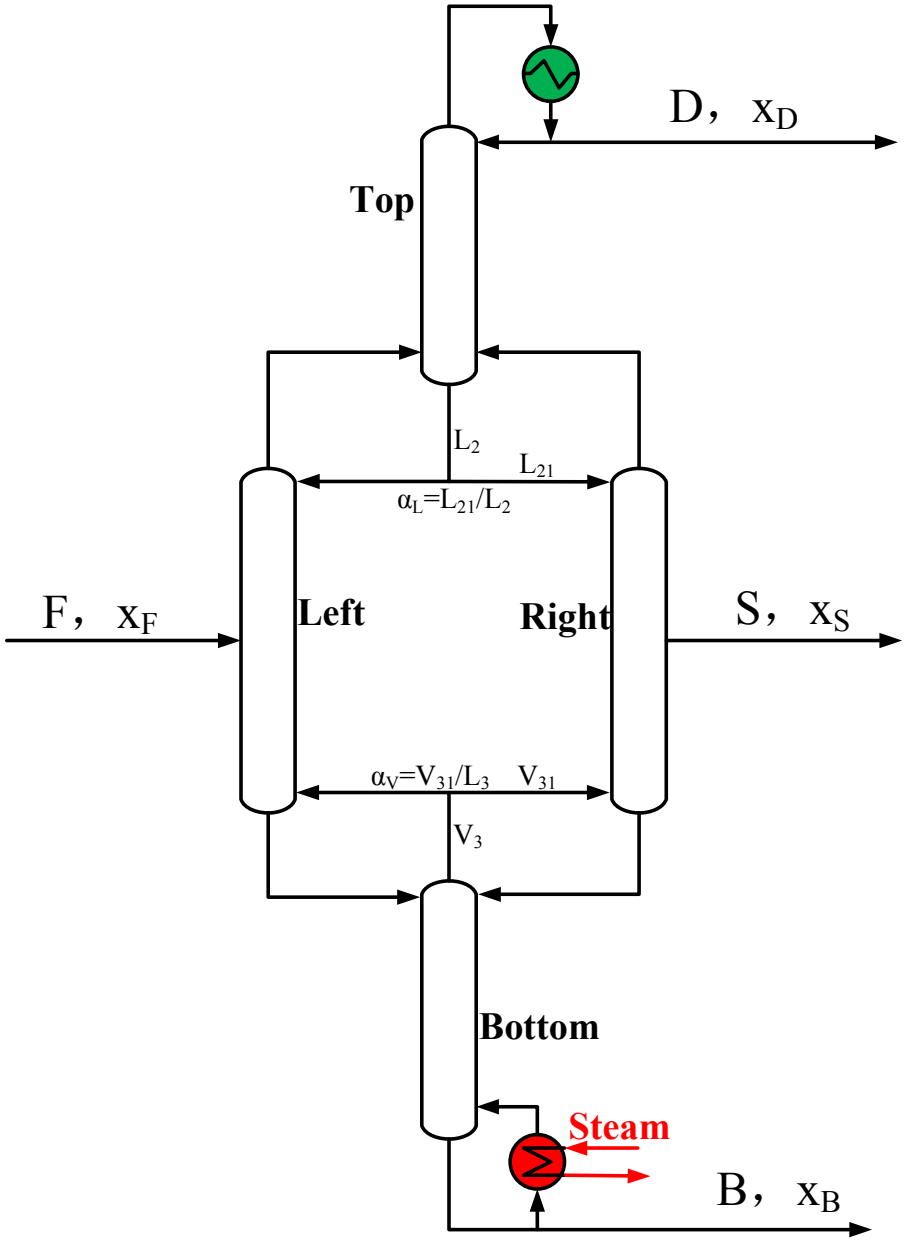

Fig S6. Four-column modules for the DWC

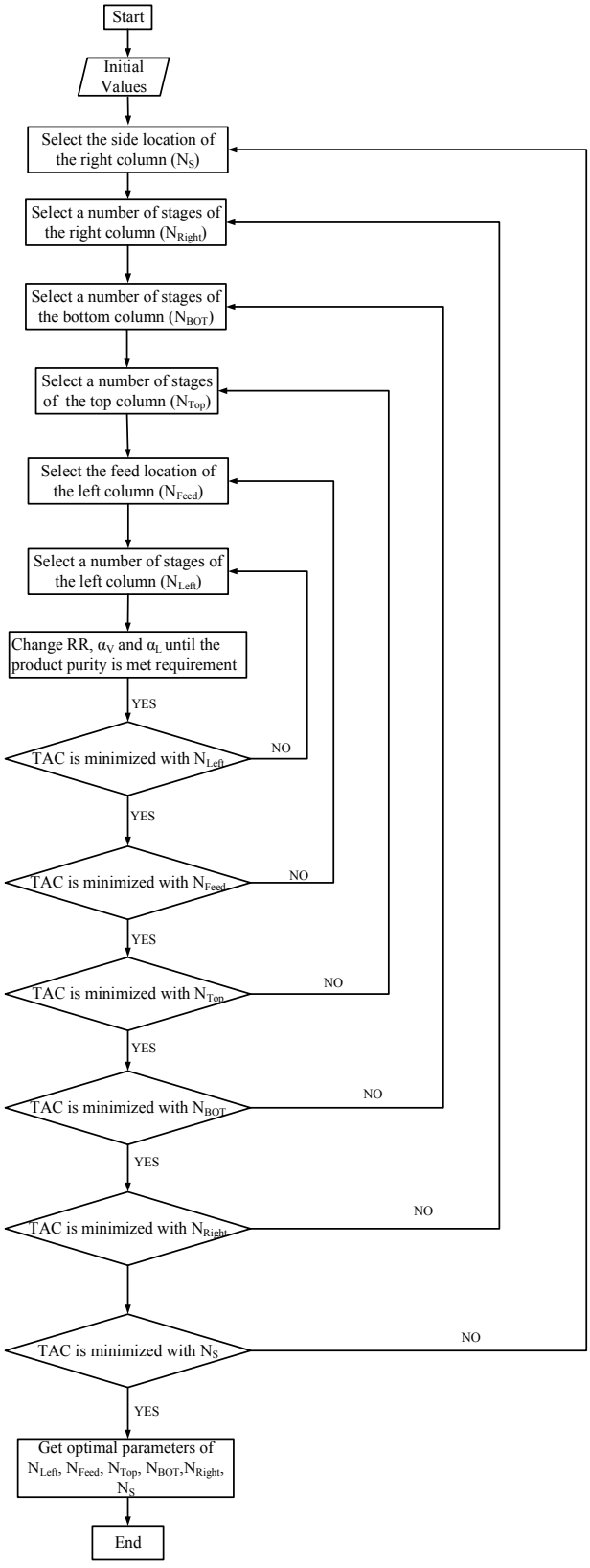

Fig S7. Sequential iterative optimization procedure of DWC

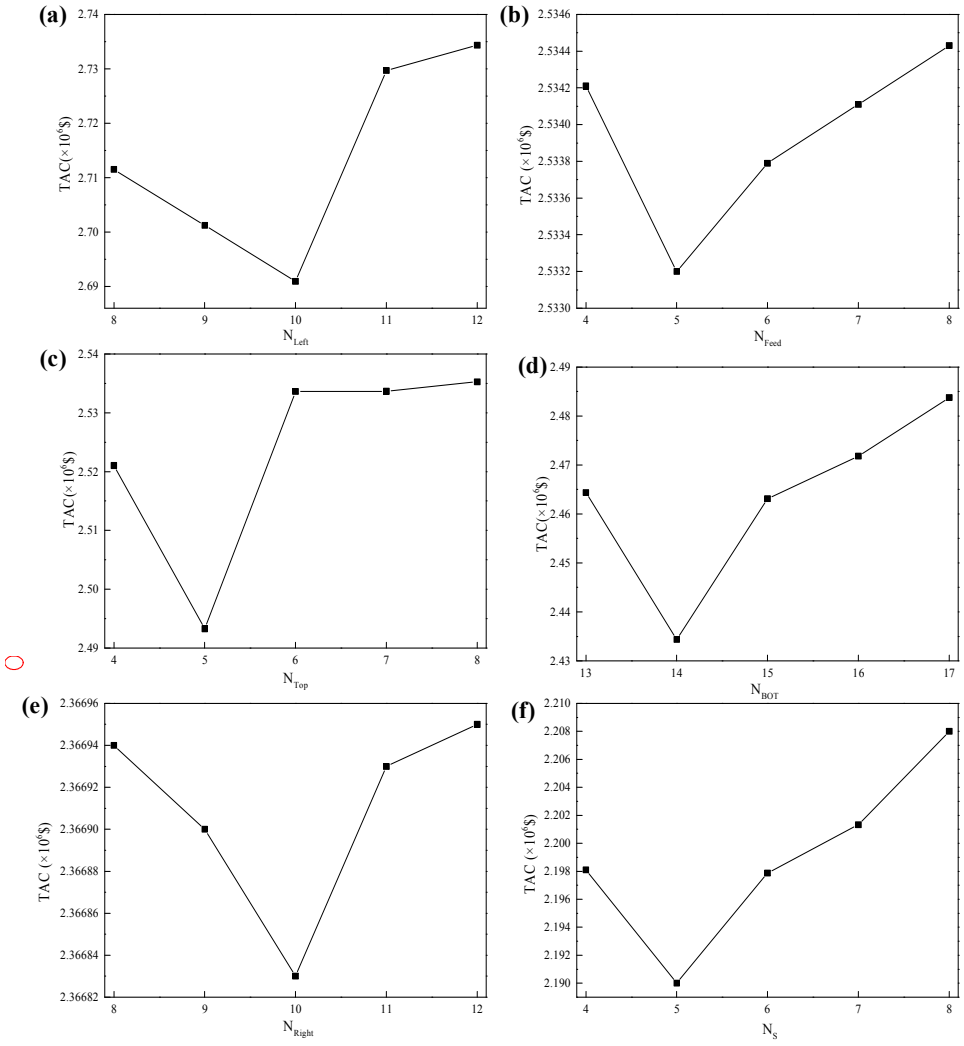

Fig S8. Optimal results of DWC

Table S6. Detailed parameters of the DWC-SHR process

Item		DWC-SHR process				
Distillation Columns						
				DWC	LPC	HPC
	Top section	Left section	Bottom section	Right section		
Reflux Ratio	7	/	/	/	7.9	14
Diameter (m)	1.431	1.415	2.207	1.440	2.763	1.794
Total Stage (N_T)	5	10	14	10	24	38
Feed Tray	/	5	/	/	13	24
Side tray	/	/	/	5	/	/
Recycled Tray	/	/	/	/	11	/
Condensers						
	Heat duty (kW)				2959.19	
C1-C	Overall heat-transfer coefficients (kW/K·m^2)				0.852	
	Heat-transfer areas (m^2)				212.66	
Self-Heat Exchangers						
	Heat duty (kW)				154.00	
E1	Overall heat-transfer coefficients (kW/K·m^2)				0.57	
	Heat-transfer areas (m^2)				5.71	
	Heat duty (kW)				326.50	
E2	Overall heat-transfer coefficients (kW/K·m^2)				0.57	
	Heat-transfer areas (m^2)				21.86	
	Heat duty (kW)				186.20	
E3	Overall heat-transfer coefficients (kW/K·m^2)				0.57	
	Heat-transfer areas (m^2)				3.63	
	Heat duty (kW)				3391.50	
E4	Overall heat-transfer coefficients (kW/K·m^2)				0.568	
	Heat-transfer areas (m^2)				959.83	
	Heat duty (kW)				417.90	
E5	Overall heat-transfer coefficients (kW/K·m^2)				0.57	
	Heat-transfer areas (m^2)				18.07	
	Heat duty (kW)				6592.17	
E6	Overall heat-transfer coefficients (kW/K·m^2)				0.568	
	Heat-transfer areas (m^2)				1093.51	
Reboilers						
		Heat duty (kW)			1667.27	
DWC-B		Overall heat-transfer coefficients (kW/K·m^2)			0.568	
		Heat-transfer areas (m^2)			48.72	
Condensers						
		Heat duty (kW)			2959.19	
DWC-C		Overall heat-transfer coefficients (kW/K·m^2)			0.852	
		Heat-transfer areas (m^2)			212.66	

Table S6. Detailed parameters of the DWC-SHR process (Continued)

Item	DWC-SHR process	
Coolers		
Cooler1	Heat duty (kW)	25.2
	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	6.16
Cooler2	Heat duty (kW)	58.3
	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	10.66
Cooler2	Heat duty (kW)	36.70
	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	10.02
Cooler2	Heat duty (kW)	131.10
	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	10.41
Cooler3	Heat duty (kW)	306.50
	Overall heat-transfer coefficients (kW/K·m^2)	0.57
	Heat-transfer areas (m^2)	17.23

Table S7. Stream energy loads of the DWC-SHR process

Stream	Stream type	Supply Tem(□)	Target Tem(□)	Duty(kW)
HPC vapor	Hot	186.4	160	7196.27
HPC Bot	Hot	167.4	70.9	154
HPC Top	Hot	160	30	356.2
DWC Bot	Hot	99.9	30	131.1
LPC vapor	Hot	72.4	56.4	3698
LPC Top	Hot	56.4	30	58.3
DWC Con	Hot	50	49.9	2959.19
DWC Top	Hot	49.9	30	25.2
HPC Reb	Cold	167	167.4	6592.17
HPC Pre	Cold	66.1	159.9	417.9
DWC Reb	Cold	99.6	99.9	1667.27
LPC Reb	Cold	65.7	65.8	3391.5
Preheater	Cold	37	108.9	666.7