A novel short process for p-xylene production based on the selectivity intensification of toluene methylation with methanol

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1.Stream data for p-xylene production process

Case 1: Ashraf's process over catalyst A

An existing PX production process proposed by Ashraf et al. [23], was used as Case 1. The detail flowsheet is shown in Figure S1, and the Material balance is in Table S1.

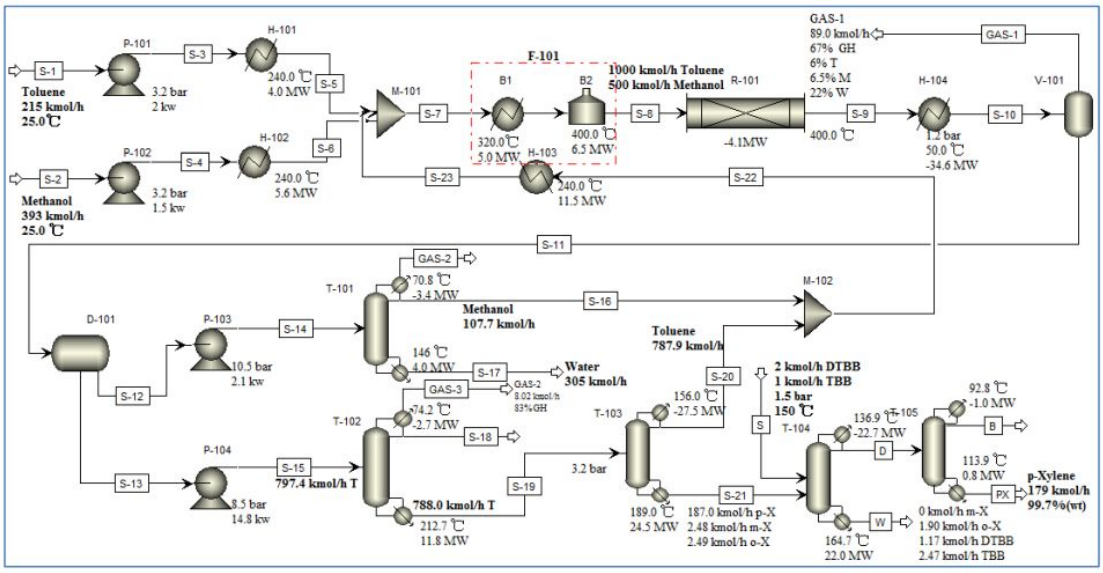

Figure.S1 flowsheet diagram for process case1

Table S1 Material balance of stream for flowsheet in Figure S1

Stream name		**S-1**	**S-2**	**S-8**	**S-10**	**GAS-1**	**S-13**	**GAS-2**	**S-16**
mole flow	kmol/h	215.24	392.62	1525.00	1606.34	89.00	1084.13	3.90	120.10
mass flow	kg/h	19832.3	12580.40	108679.3	108679.3	2679.93	98160.10	114.74	3948.35
vapor fraction		0	0	1	0.04	1	0	1	0
temperature	℃	25.00	25.00	400.00	50.00	47.24	46.00	70.77	70.77
pressure	bar	1.00	1.00	3.00	2.00	1.00	1.20	4.00	4.00
Component Mole Flow									
Toluene	kmol/h	215.24	0.00	1000.89	805.65	6.67	797.38	0.01	1.59
Methanol	kmol/h	0.00	392.62	500.00	173.72	5.18	55.40	1.21	107.72
p-X	kmol/h	0.00	0.00	12.11	199.74	0.45	199.15	0.00	0.14
Water	kmol/h	0.00	0.00	9.43	340.26	17.90	7.67	0.04	43.10
Benzene	kmol/h	0.00	0.00	1.92	8.44	0.14	8.28	0.00	0.02
GH	kmol/h	0.00	0.00	0.98	73.35	60.64	9.10	2.63	0.98
m-X	kmol/h	0.00	0.00	0.14	2.63	0.01	2.62	0.00	0.00
o-X	kmol/h	0.00	0.00	0.05	2.54	0.00	2.52	0.00	0.02
TBB	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DTBB	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TBMX	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Stream name		**S-19**	**S-21**	**S-22**	**S**	**GAS-3**	**W**	**B**	**PX**
mole flow	kmol/h	994.12	192.12	920.10	3	8.02	7.63	8.50	179.0
mass flow	kg/h	9438.0	20397.4	77988.9	514.88	238.85	1052.16	856.8	19003.3
vapor fraction		0	0	1	0	1	0	0	0
temperature	℃	212.71	189.0	136.11	150.00	74.25	164.70	92.83	113.88
pressure	bar	8.20	3.30	3.00	1.50	8.00	1.05	0.48	0.50
Component Mole Flow									
Toluene	kmol/h	787.96	0.00	787.90	0.00	0.09	0.00	0.00	0.00
Methanol	kmol/h	0.00	0.00	107.70	0.00	1.21	0.00	0.00	0.00
p-X	kmol/h	199.13	187.15	22.12	0.00	0.00	1.89	6.87	178.40
Water	kmol/h	0.00	0.00	9.43	0.00	0.11	0.00	0.00	0.00
Benzene	kmol/h	1.89	0.00	1.92	0.00	0.10	0.00	1.63	0.02
GH	kmol/h	0.00	0.00	0.98	0.00	6.58	0.00	0.00	0.00
m-X	kmol/h	2.62	2.48	0.14	0.00	0.00	0.00	0.00	0.01
o-X	kmol/h	2.52	2.49	0.05	0.00	0.00	1.90	0.01	0.57
TBB	kmol/h	0.00	0.00	0.00	1.00	0.00	0.18	0.00	0.00
DTBB	kmol/h	0.00	0.00	0.00	2.00	0.00	1.17	0.00	0.00
TBMX	kmol/h	0.00	0.00	0.00	0.00	0.00	2.47	0.00	0.00

Case 2: Modified Ashraf's process over catalyst B

The modified process by using the reaction kinetics model for catalyst B in the reaction stage on the basis of Ashraf's process was denoted as Case 2 and shown in Figure S2. The according Material balance is in Table S2.

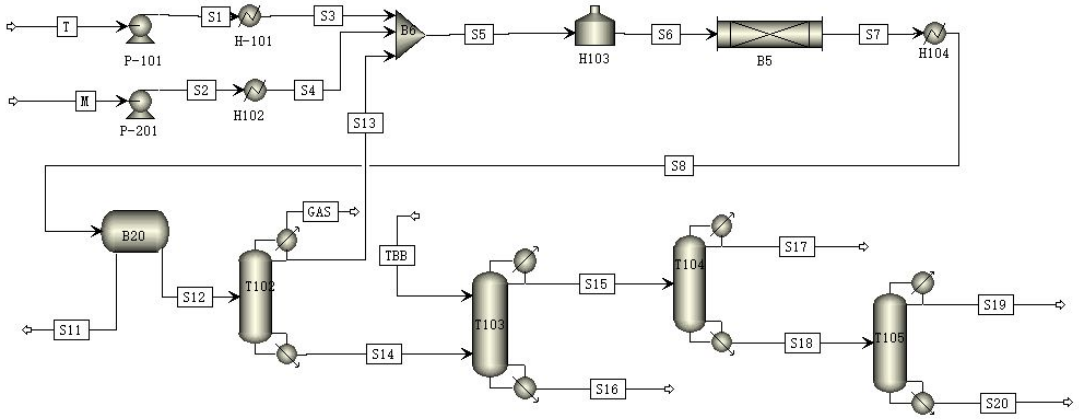

Figure.S2 flowsheet diagram for process case2

Table S2 Material balance of stream for flowsheet in Figure S2

	GAS	**M**	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S11**
T,°C	133.13	25.00	25.35	25.30	150.00	420.00	126.22	420.00	482.79	50.00	48.09
P,bar	3.00	1.01	5.01	5.01	3.00	4.00	3.00	4.00	4.00	4.00	4.00
Vapor Fraction	1.00	0.00	0.00	0.00	0.00	1.00	0.33	1.00	1.00	0.00	0.00
Mole flows, kmol/hr	1.45	197.00	193.00	197.00	193.00	197.00	1115.52	1115.52	1115.52	1115.52	196.46
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C_2H_4	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.03	0.03	0.03	0.00
Methanol	0.00	197.00	0.00	197.00	0.00	197.00	197.00	197.00	0.00	0.00	0.00
Toluenen	0.92	0.00	193.00	0.00	193.00	0.00	916.91	916.91	725.38	725.38	0.00
OX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.17	3.17	0.00
PX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	180.14	180.14	0.00
MX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.74	2.74	0.00
TMB	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.48	5.48	0.00
WATER	0.54	0.00	0.00	0.00	0.00	0.00	1.58	1.58	198.58	198.58	196.46
1:4-D-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TERT--01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-TER-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S12	**S13**	**S14**	**S15**	**S16**	**S17**	**S18**	**S19**	**S20**	**T**	**TBB**
T, °C	48.09	133.13	184.74	85.09	137.68	136.23	184.64	165.66	203.32	25.00	150.00
P, bar	4.00	3.00	3.00	0.20	0.20	3.00	3.00	2.00	3.00	1.01	1.50
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole flows, kmol/h	919.05	725.52	192.08	190.22	10.26	5.14	185.08	178.68	6.40	193.00	8.40
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C_2H_4	0.03	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Toluene	725.38	723.91	0.56	0.56	0.00	0.45	0.11	0.11	0.00	193.00	0.00
OX	3.17	0.00	3.17	3.17	0.00	0.00	3.17	0.08	3.09	0.00	0.00

PX	180.14	0.00	180.14	180.14	0.00	1.61	178.53	178.35	0.18	0.00	0.00
MX	2.74	0.00	2.74	0.14	0.00	0.00	0.14	0.14	0.00	0.00	0.00
TMB	5.48	0.00	5.48	2.21	3.26	0.00	2.21	0.00	2.21	0.00	0.00
WATER	2.11	1.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1:4-D-01	0.00	0.00	0.00	0.47	4.41	0.00	0.47	0.00	0.47	0.00	4.40
TERT--01	0.00	0.00	0.00	0.45	0.00	0.00	0.45	0.00	0.45	0.00	4.00
5-TER-01	0.00	0.00	0.00	0.00	2.59	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	0.00	0.00	3.07	0.00	3.07	0.00	0.00	0.00	0.00	0.00

Case 3: Liu's process over catalyst A

An existing PX production process proposed by Liu et al. [6] was used for Case 3 (Figure S3), which eliminated the methanol recovery tower T-100 and recycling system. And the according Material balance is in Table S3.

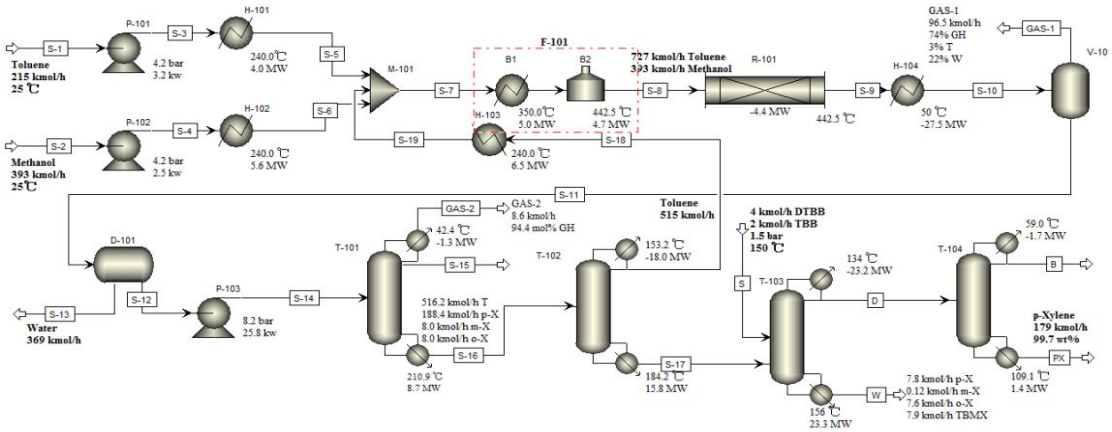

Figure.S3 flowsheet diagram for process case3

Table S3 Material balance of stream for flowsheet in Figure S3

Stream		**S-1**	**S-2**	**S-7**	**S-9**	**GAS-1**	**S-14**	**GAS-2**
mole flow	kmol/h	215.24	393.00	1132.74	1226.93	96.87	750.58	8.61
mass flow	kg/h	19832.30	12592.60	80633.10	80633.10	2728.20	70932.70	252.59
vapor fraction		0.00	0.00	1.00	1.00	1.00	0.00	0.00
temperature	°C	25.00	25.00	240.00	442.50	25.00	21.00	42.44
pressure	bar	1.00	1.00	4.00	4.00	1.10	8.20	8.00
Component Mole Flow								
Toluene	kmol/h	215.24	0.00	727.29	515.56	1.82	513.69	0.00
Methanol	kmol/h	0.00	393.00	393.00	8.40	0.12	2.09	0.09
p-X	kmol/h	0.00	0.00	1.90	189.58	0.23	189.34	0.00
Water	kmol/h	0.00	0.00	0.00	384.60	13.50	2.23	0.15
Benzene	kmol/h	0.00	0.00	10.49	18.24	0.20	18.03	0.24
GH	kmol/h	0.00	0.00	0.00	94.19	80.97	8.84	8.13
m-X	kmol/h	0.00	0.00	0.06	8.21	0.01	8.20	0.00
o-X	kmol/h	0.00	0.00	0.01	8.16	0.01	8.15	0.00
TBB	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DTBB	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TBMX	kmol/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Stream name		**S-15**	**S-17**	**S-19**	**S**	**W**	**B**	**PX**
mole flow	kmol/h	12.39	205.08	524.50	6.00	23.57	8.50	179.00
mass flow	kg/h	718.61	21753.30	48208.20	914.54	2951.12	716.70	19003.00
vapor fraction		0	0.00	1.00	0.00	1.00	0.00	0.00
temperature	°C	21.09	184.25	240.00	150.00	156.19	59.00	109.05
pressure	bar	8	3.00	4.00	1.50	1.06	0.40	0.43
Component Mole Flow								
Toluene	kmol/h	0.29	1.35	512.05	0.00	0.00	1.28	0.07
Methanol	kmol/h	2	0.00	0.00	0.00	0.00	0.00	0.00
p-X	kmol/h	0	187.44	1.90	0.00	7.84	1.24	178.37
Water	kmol/h	2.08	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	kmol/h	7.31	0.00	10.48	0.00	0.00	5.98	0.00
GH	kmol/h	0.71	0.00	0.00	0.00	0.00	0.00	0.00
m-X	kmol/h	0	8.14	0.06	0.10	0.15	0.00	0.02
o-X	kmol/h	0	8.14	0.01	0.00	7.60	0.00	0.50
TBB	kmol/h	0	0.00	0.00	4.00	0.01	0.00	0.00
DTBB	kmol/h	0	0.00	0.00	2.00	0.01	0.00	0.00
TBMX	kmol/h	0	0.00	0.00	0.00	7.97	0.00	0.00

Case 4: Modified Liu's process over catalyst B

The modified process by using the reaction kinetics model for catalyst B in the reaction stage on the basis of Liu's process was denoted as Case 4 and shown in Figure S4. The according Material balance is in Table S4.

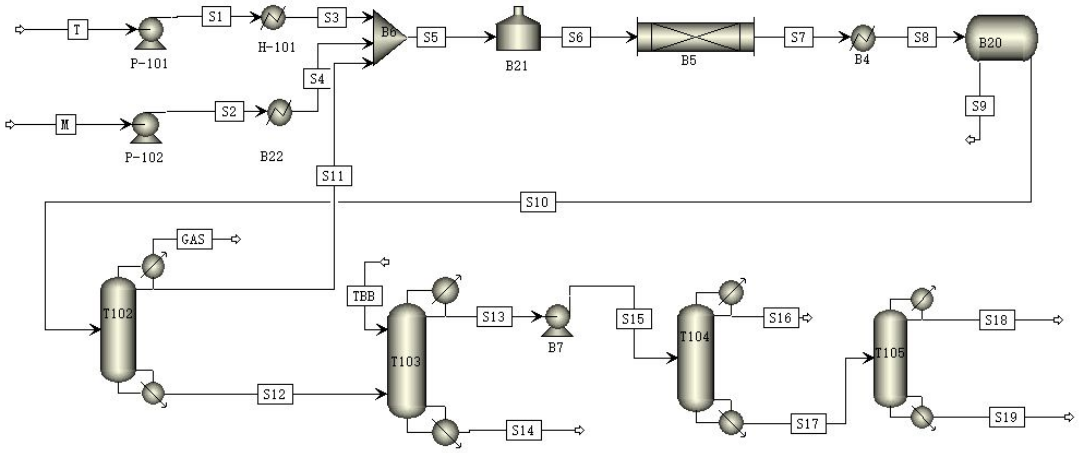

Figure.S4 flowsheet diagram for process case4

Table S4 Material balance of stream for flowsheet in Figure S4

	GAS	**M**	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**
T, °C	133.75	25.00	25.35	25.30	150.00	420.00	126.39	442.50	503.87	50.00	48.13	48.13
P, bar	3.00	1.01	5.01	5.01	3.00	4.00	3.00	4.00	4.00	4.00	4.00	4.00
Vapor Fraction	1.00	0.00	0.00	0.00	0.00	1.00	0.33	1.00	1.00	0.00	0.00	0.00
Mole flows kmol/hr	1.68	197.00	194.00	197.00	194.00	197.00	1119.48	1119.48	1119.48	1119.48	196.40	923.08
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C_2H_4	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.00	0.02
Methanol	0.00	197.00	0.00	197.00	0.00	197.00	197.00	197.00	0.00	0.00	0.00	0.00
Toluenen	1.08	0.00	194.00	0.00	194.00	0.00	920.93	920.93	729.03	729.03	0.00	729.03
OX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.58	3.58	0.00	3.58
PX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	180.16	180.16	0.00	180.16
MX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.08	3.08	0.00	3.08
TMB	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.10	5.10	0.00	5.10
WATER	0.60	0.00	0.00	0.00	0.00	0.00	1.52	1.52	198.52	198.52	196.40	2.12
1:4-D-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TERT--01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5-TER-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	S11	**S12**	**S13**	**S14**	**S15**	**S16**	**S17**	**S18**	**S19**	**T**	**TBB**	
T, °C	133.75	184.61	84.90	138.04	85.00	133.52	184.60	184.07	201.84	25.00	150.00	
P, bar	3.00	3.00	0.20	0.20	3.00	3.00	3.00	3.00	3.00	1.01	1.50	
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
Mole flows kmol/hr	728.48	192.92	191.02	10.31	191.02	5.32	185.90	179.17	6.53	194.00	8.40	
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
C_2H_4	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
Methanol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
Toluenen	726.93	1.02	1.02	0.00	1.02	0.99	0.03	0.03	0.00	194.00	0.00	

OX	0.00	3.58	3.58	0.00	3.58	0.00	3.58	0.31	3.27	0.00	0.00	
PX	0.00	180.15	180.15	0.00	180.15	1.10	179.05	178.66	0.39	0.00	0.00	
MX	0.00	3.08	0.18	0.00	0.18	0.00	0.18	0.18	0.00	0.00	0.00	
TMB	0.00	5.10	1.94	3.15	1.94	0.00	1.94	0.00	1.94	0.00	0.00	
WATER	1.52	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
1:4-D-01	0.00	0.00	0.47	4.26	0.47	0.00	0.47	0.00	0.47	0.00	4.40	
TERT--01	0.00	0.00	0.45	0.00	0.45	0.00	0.45	0.00	0.45	0.00	4.00	
5-TER-01	0.00	0.00	0.00	2.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
Benzene	0.00	0.00	3.23	0.00	3.23	3.23	0.00	0.00	0.00	0.00	0.00	

Case 5: Short process over catalyst A

The proposed short processes using catalysts A was presented in the Figure S5, which retained the methanol recovery tower (T-100) and recycling system but removed the reactive distillation tower (T-103). The according Material balance is in Table S5.

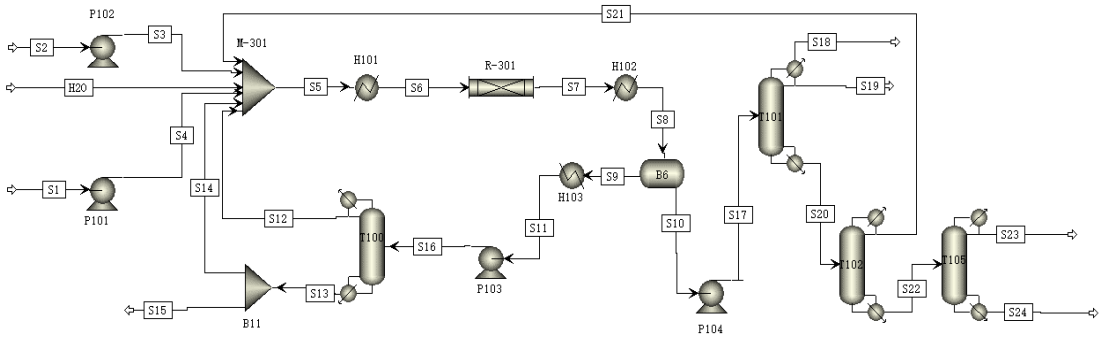

Figure.S5 flowsheet diagram for process case5

Table S5 Material balance of stream for flowsheet in Figure S5

	H_2O	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**
T, °C	25.00	25.00	25.00	25.10	25.17	45.37	442.50	442.50	40.00	1.00	1.00	70.00	89.87
P, bar	3.00	1.00	1.00	3.00	3.00	1.00	4.00	4.00	4.00	1.00	1.00	3.00	3.00
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00
Mole flows kmol/hr	2000.00	207.00	257.00	257.00	207.00	9462.88	9462.88	9495.24	9495.24	5790.12	3705.12	5790.12	324.39
C_2H_4	0.00	0.00	0.00	0.00	0.00	1.00	1.00	33.37	33.37	1.00	32.36	1.00	1.00
Methanol	0.00	0.00	257.00	257.00	0.00	566.17	566.17	334.05	334.05	309.92	24.13	309.92	308.07
Benzene	0.00	0.00	0.00	0.00	0.00	12.35	12.35	24.23	24.23	0.02	24.21	0.02	0.02
Toluene	0.00	207.00	0.00	0.00	207.00	3633.74	3633.74	3442.59	3442.59	1.69	3440.90	1.69	1.69
OX	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.61	0.00	0.61	0.00	0.00
PX	0.00	0.00	0.00	0.00	0.00	1.17	1.17	179.22	179.22	0.02	179.20	0.02	0.02
MX	0.00	0.00	0.00	0.00	0.00	0.24	0.24	0.86	0.86	0.00	0.86	0.00	0.00
WATER	2000.00	0.00	0.00	0.00	0.00	5248.20	5248.20	5480.31	5480.31	5477.46	2.86	5477.46	13.59
	S13	**S14**	**S15**	**S16**	**S17**	**S18**	**S19**	**S20**	**S21**	**S22**	**S23**	**S24**	
T, °C	133.52	133.52	133.52	70.00	1.05	64.96	64.96	111.10	110.06	137.90	137.88	142.29	
P, bar	3.00	3.00	3.00	3.00	2.20	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	
Mole flows kmol/hr	5465.73	3235.71	2230.02	5790.12	3705.12	85.33	1.74	3618.05	3438.98	179.67	178.83	0.85	
C_2H_4	0.00	0.00	0.00	1.00	32.36	32.34	0.02	0.00	0.00	0.00	0.00	0.00	
Methanol	1.86	1.10	0.76	309.92	24.13	24.06	0.07	0.00	0.00	0.00	0.00	0.00	
Benzene	0.00	0.00	0.00	0.02	24.21	11.52	0.37	12.32	12.32	0.00	0.00	0.00	
Toluene	0.00	0.00	0.00	1.69	3440.90	14.56	1.29	3425.06	3425.06	0.00	0.00	0.00	
OX	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.61	0.00	0.61	0.00	0.61	
PX	0.00	0.00	0.00	0.02	179.20	0.00	0.00	179.20	1.16	178.65	178.42	0.23	
MX	0.00	0.00	0.00	0.00	0.86	0.00	0.00	0.86	0.44	0.41	0.41	0.03	
WATER	5463.87	3234.61	2229.26	5477.46	2.86	2.85	0.00	0.00	0.00	0.00	0.00	0.00	

Case 6: Short process over catalyst B

The proposed short processes using catalysts B was presented in the Figure S6, which removed both the benzene tower (T-101) and the reactive distillation tower (T-103). The according Material balance is in Table S6.

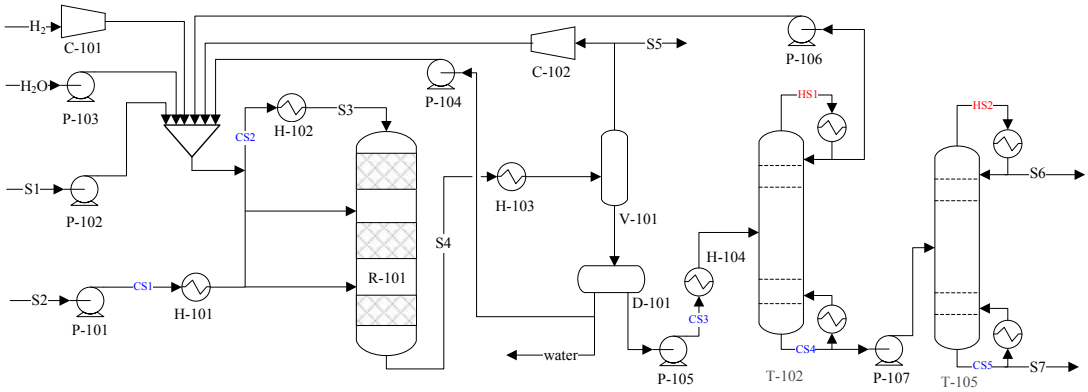

Figure.S6 flowsheet diagram for process case6

Table S6 Material balance of stream for flowsheet in Figure S6

	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
T, ℃	25.00	25.00	25.00	25.00	470.00	478.40	40.00	27.00	165.65	224.53
P, kPa	100.00	100.00	100.00	100.00	350.00	350.00	300.00	300.00	200.00	400.00
Vapor Fraction	1.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00	0.00	0.00
Mole Flows ($kmol \cdot h^{-1}$)	90.00	2371.00	185.50	187.00	9448.66	9579.56	95.09	2555.18	179.13	4.12
H_2	90.00	0.00	0.00	0.00	907.68	907.68	90.00	0.00	0.00	0.00
C_2H_4	0.00	0.00	0.00	0.00	0.06	0.06	0.00	0.00	0.00	0.00
M	0.00	0.00	0.00	187.00	70.90	14.82	0.02	0.00	0.00	0.00
T	0.00	0.00	185.50	0.00	1523.41	1340.26	2.20	0.00	0.15	0.00
OX	0.00	0.00	0.00	0.00	0.00	0.24	0.00	0.00	0.12	0.12
PX	0.00	0.00	0.00	0.00	0.56	179.39	0.06	0.00	178.59	0.18
MX	0.00	0.00	0.00	0.00	0.00	0.27	0.00	0.00	0.27	0.00
TMB	0.00	0.00	0.00	0.00	0.00	3.82	0.00	0.00	0.00	3.82
H_2O	0.00	2371.00	0.00	0.00	6946.05	7133.03	2.81	2555.18	0.00	0.00

2 Heat integration for six cases

Case 1: Ashraf's process over catalyst A

The process flow data and results for heat integration information of case 1 were shown in Table S7, Figure S7and Figure S8.

Table S7 process flow data for Case1

Stream	Temperature ℃		Enthalpy, MW
	in	out	
S9-S10	400.00	50.00	34.58
S22-S23	136.10	240.00	11.55
S3-S5	25.00	240.00	4.01
S4-S6	25.00	240.00	5.60
S7-S8	240.00	400.00	10.37
T1-D	105.80	70.80	3.36
T1-W	145.80	145.90	3.99
T2-D	142.80	74.20	2.73
T2-W	211.50	212.70	11.81
T3-D	156.40	156.00	27.52
T3-W	188.80	189.00	24.49
T4-D	137.80	136.90	22.69
T4-W	147.40	164.70	22.06
T5-D	107.30	92.80	0.92
T5-W	113.80	113.90	0.65

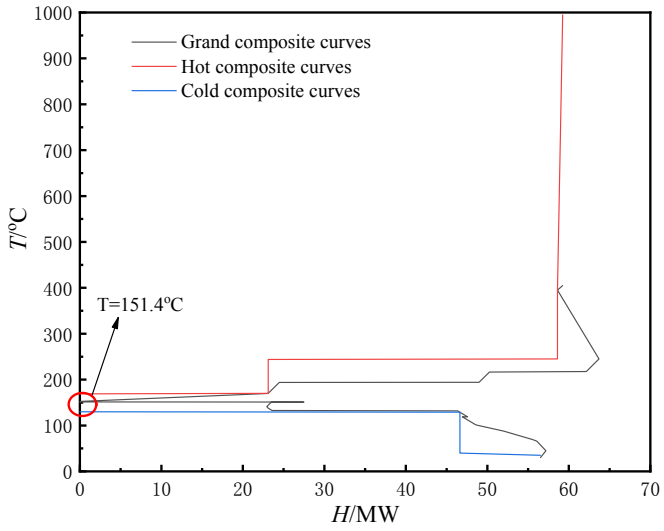

Figure.S7 the composite curve of cold and hot logistics in the process for Case1

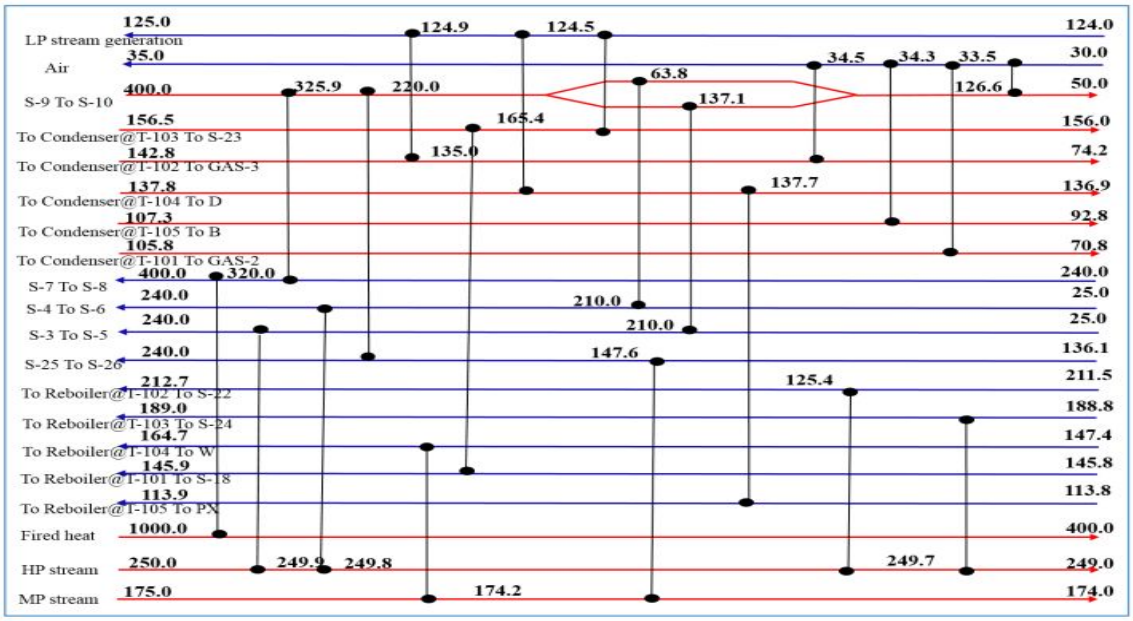

Figure.S8 The HEN diagram for the process of Case1

Case 2: Modified Ashraf's process over catalyst B

The process flow data and results for heat integration information of case 2 were shown in Table S8, Figure S9 and Figure S10.

Table S8 process flow data for Case2

Stream	Temperature ℃		Enthalpy, MW
	in	out	
S2-S4	25.30	420.00	3.35
S7-S8	482.79	50.00	33.01
S5-S6	126.23	420.00	21.16
S1-S3	25.35	150.00	1.18
T105-W	202.82	203.32	16.70
T105-D	166.16	165.66	16.93
T104-D	153.79	136.23	0.96
T103-W	119.13	137.68	19.00
T102-W	184.39	184.74	23.00
T102-D	153.73	133.16	18.30
T103-D	87.13	85.09	19.93
T104-W	184.48	184.64	2.15

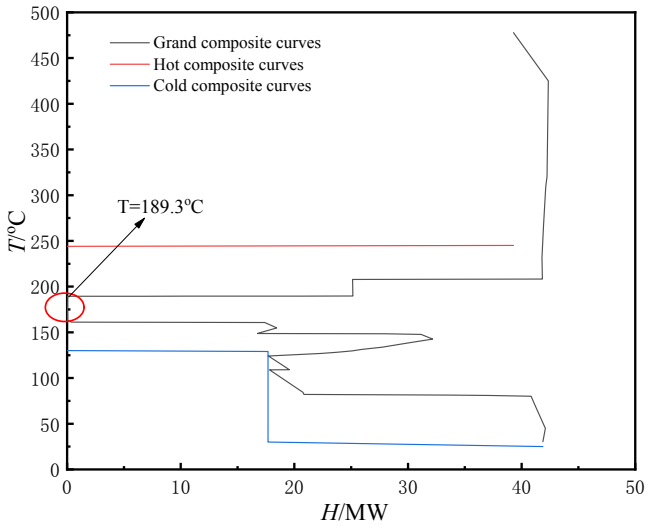

Figure.S9 the composite curve of cold and hot logistics in the process for Case2

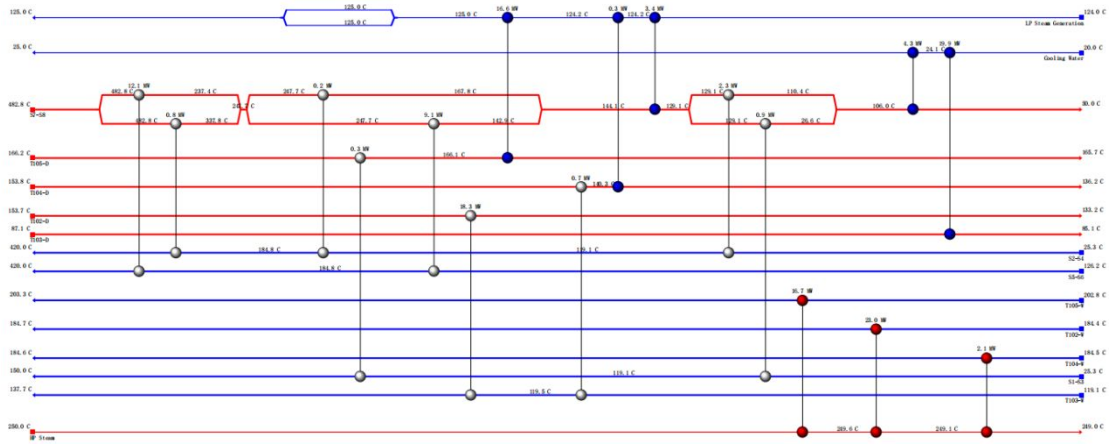

Figure.S10 The HEN diagram for the process of Case2

Case 3: Liu's process over catalyst A

The process flow data and results for heat integration information of case 3 were shown in Table S9, Figure S11 and Figure S12.

Table S9 process flow data for Case3

Stream	Temperature ℃		Enthalpy, MW
	in	out	
S9-S10	442.50	50.00	27.55
S3-S5	25.00	240.00	4.00
S4-S6	25.00	240.00	5.63
S18-S19	153.20	240.00	6.53
S7-S8	240.00	442.50	9.81
V101Heat	50.00	25.00	0.98
T1-D	147.20	42.40	1.27
T1-W	209.00	210.90	8.66
T2-D	153.70	153.20	17.99
T2-W	184.00	184.20	15.81
T3-D	137.00	133.90	22.97

T3-W	145.70	156.20	22.34
T4-D	73.70	59.00	2.01
T4-W	108.90	109.10	1.72

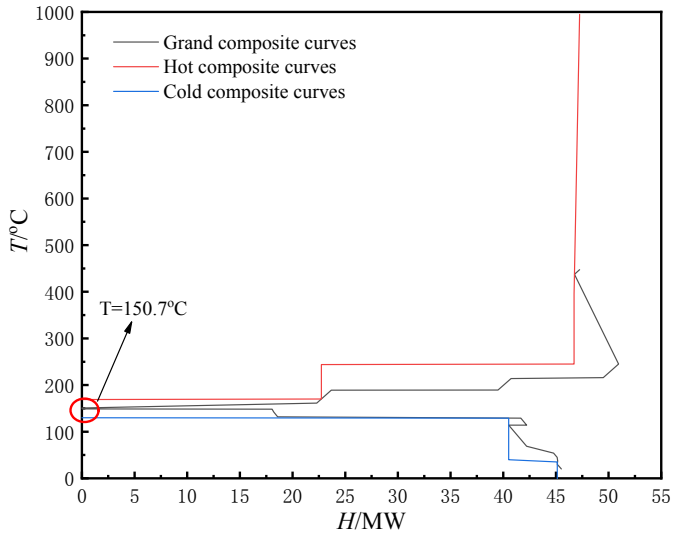

Figure.S11 the composite curve of cold and hot logistics in the process for Case3

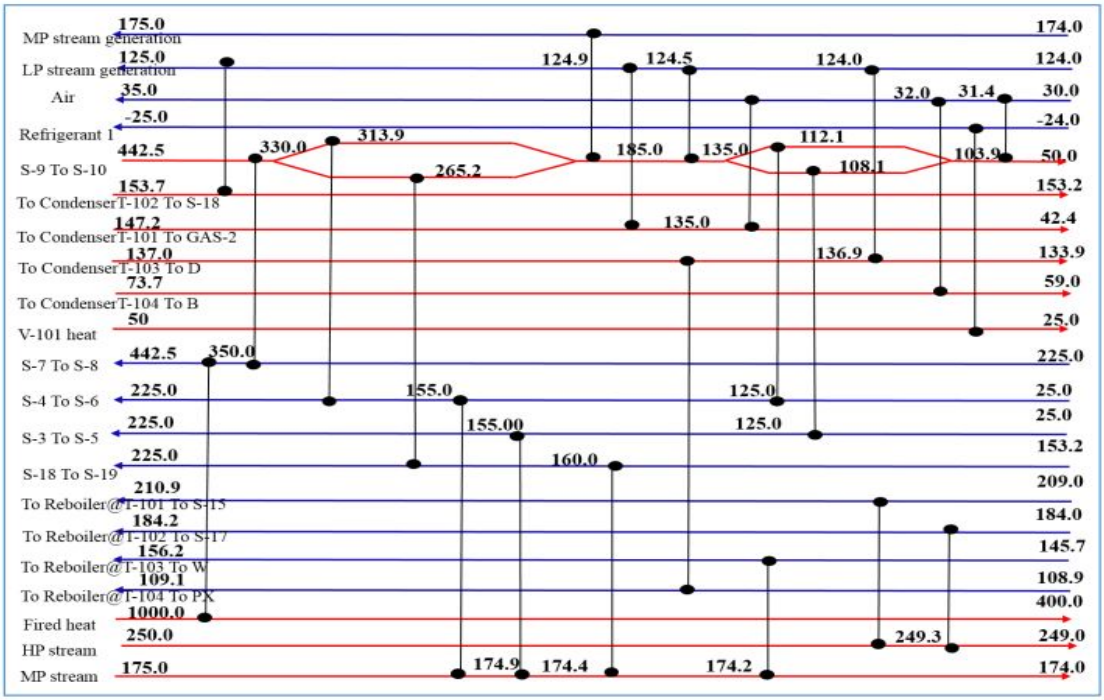

Figure.S12 The HEN diagram for the process of Case3

Case 4: Modified Liu's process over catalyst B

The process flow data and results for heat integration information of case 4 were shown in Table S10, Figure S13 and Figure S14.

Table S10 process flow data for Case4

Stream	Temperature ℃		Enthalpy, MW
	in	out	
S2-S4	25.30	420.00	3.35
S7-S8	504.16	50.00	34.32
S5-S6	126.37	442.50	22.45
S1-S3	25.35	150.00	1.18
T105-W	201.83	202.33	16.66
T105-D	166.18	165.68	16.88
T104-D	155.21	136.02	0.96
T103-W	119.67	138.15	18.98
T102-W	184.55	184.81	23.00
T102-D	153.73	133.77	18.28
T103-D	87.12	85.10	19.92
T104-W	184.50	184.65	2.15

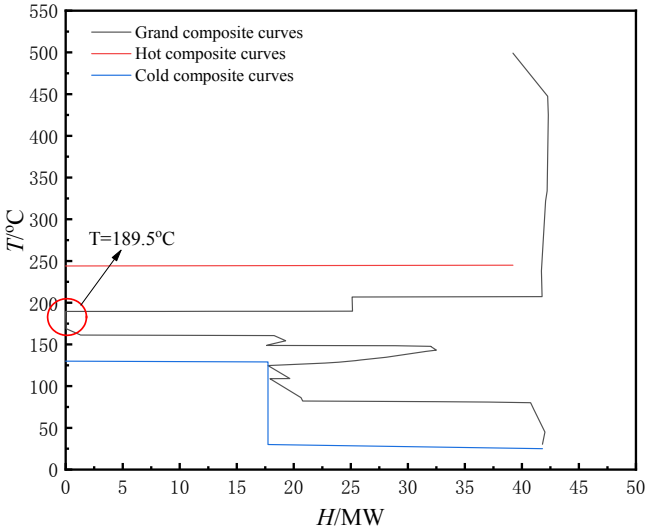

Figure.S13 the composite curve of cold and hot logistics in the process for Case4

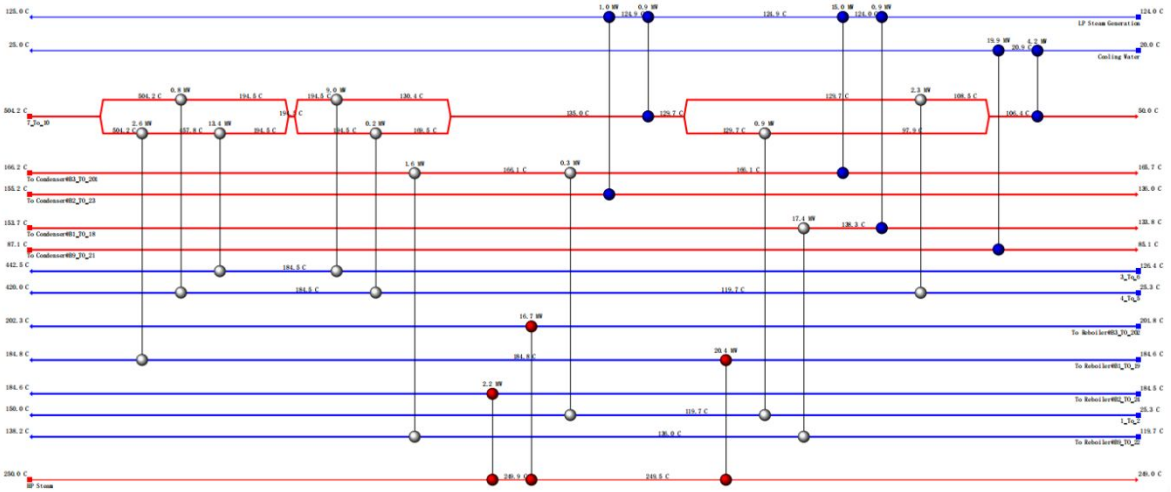

Figure.S14 The HEN diagram for the process of Case4

Case 5: Short process over catalyst A

The process flow data and results for heat integration information of case 5 were shown in Table S11, Figure S15 and Figure S16.

Table S11 process flow data for Case5

Stream	Temperature ℃		Enthalpy,MW
	in	out	
S9-	25.00	70.00	7.81
S5-S6	44.89	442.50	181.07
S7-S8	442.50	40.00	193.13
T3-D	138.38	137.88	15.09
T3-W	141.91	142.41	15.09
T4-D	96.40	89.86	13.49
T1-W	110.79	111.11	22.76
T2-W	137.90	138.50	67.00
T1-D	98.28	64.25	3.82
T4-W	133.40	133.52	21.35
T2-D	110.20	109.00	77.00

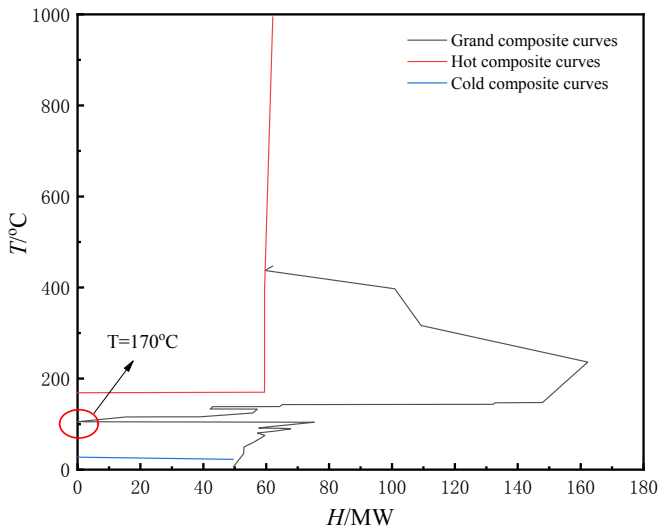

Figure.S15 the composite curve of cold and hot logistics in the process for Case5

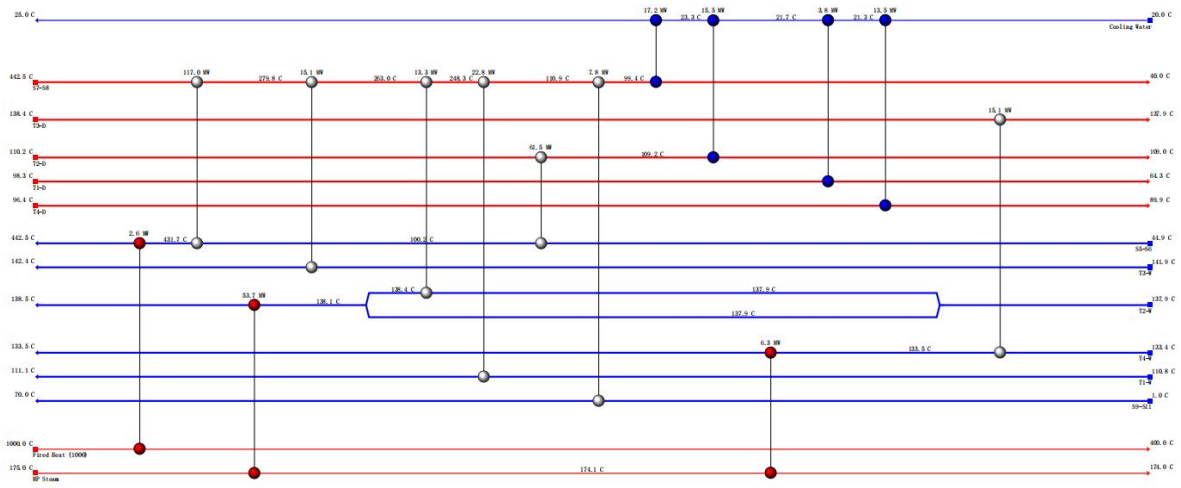

Figure.S16 The HEN diagram for the process of Case5

Case 6: Short process over catalyst B

The process flow data and results for heat integration information of case 1 were shown in Table S12, Figure S17 and Figure S18.

Table S12 process flow data for Case6

Stream	Temperature ℃		Enthalpy, MW
	in	out	
CS1	25.00	90.00	0.39
CS2	77.00	470.00	147.20
CS3	28.90	150.00	11.06
CS4	165.90	166.10	27.80
CS5	224.00	224.50	8.74
HS1	479.00	40.00	171.20
HS2	136.10	135.50	18.46
HS3	166.20	165.70	8.73

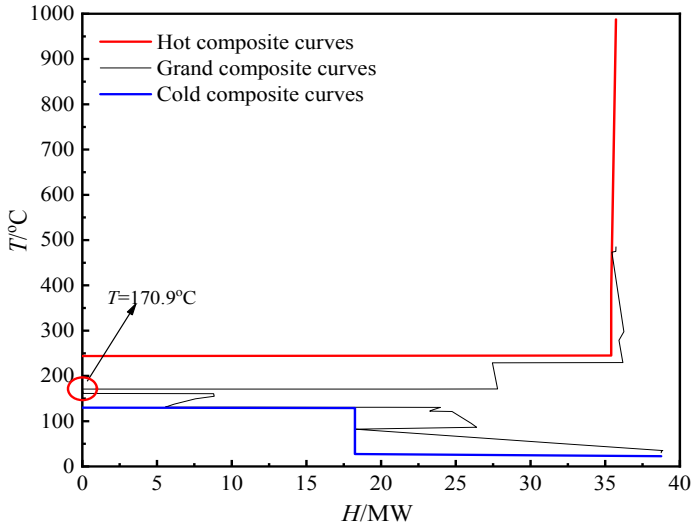

Figure.S17 the composite curve of cold and hot logistics in the process for Case6

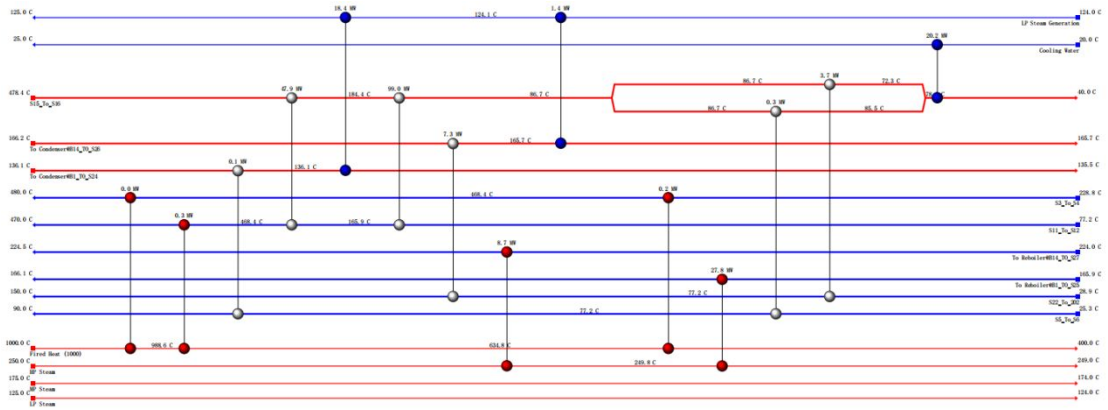

Figure.S18 The HEN diagram for the process of Case6