Supporting Materials

Computer-aided multi-objective optimization integrated with multi-dimensional assessment for the offshore oil to chemical process

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1. Process simulation and modeling strategy

1.1. Molecular reconstruction of offshore crude oil in Aspen HYSYS

For the catalytic cracking process of crude oil, since the twenty-one lumped reaction kinetics still has a severe lack of ability to describe the lumped light hydrocarbons and naphtha, the application of this method to modeling will lead to a significant deviation in the calculation of product distribution and properties of light hydrocarbons such as naphtha in the high-temperature catalytic cracking process. In contrast, the molecular composition lumped kinetic model can better predict the distribution and properties of naphtha catalytic cracking products. However, because the number of molecular compositions lumped increases significantly with the widening of the final distillation point, the complexity of the model is increased dramatically, and the calculation efficiency is reduced considerably. Based on comprehensive analysis, depending on the advantages of the zonal reaction of our research group's two-stage riser catalytic cracking reactor, different reaction zones can be set for light hydrocarbons such as naphtha and heavy oil fractions (see Fig. 6b).

Therefore, we propose a new modeling strategy to establish a two-stage riser catalytic cracking reaction kinetics model with different molecular levels (naphtha, kerosene, diesel) and distillate structure blocks (heavy oil) for the complex crude oil direct catalytic cracking reaction system. This strategy can take not only advantage of the effective solution and accurate prediction of the lumped reaction kinetic model (the enhanced model of heavy oil feedstock solving efficiency) but also realize the modeling of light fraction catalytic cracking processes such as naphtha and diesel oil by using the molecular level model (the enhanced model description ability reaches the molecular level). Based on the process integration model, the yield and properties of key products from direct catalytic cracking of crude oil were calculated and predicted. The previous research results show that the average relative error between the simulation value and the experimental value of our model is less than 5%.

As shown in Fig. 6a, the first step to establish a molecular level model for the two-stage riser catalytic cracking process of offshore low sulfur paraffinic crude oil is to use

crude oil molecular reconstruction technology to reconstruct the light fraction of crude oil at the molecular level. First, the properties of crude oil at the molecular level are obtained based on analytical chemistry. Next, the light fraction of crude oil is sampled randomly by the Monte Carlo method to obtain virtual molecules. According to the mixing law of crude oil molecular properties, the properties of the pseudo molecular mixtures are obtained. The group contribution method calculates the molecular density and boiling point. Then, the acquired overall molecular properties are compared with the calibration data of crude oil, and the property optimization objective function is constructed. The simulated annealing optimization algorithm optimizes the objective function to achieve the specified optimization goal. The initial molecular composition of the light fraction of offshore paraffinic crude oil can be determined by performing the above series of steps.

Based on the molecular reconstruction strategy of offshore crude oil proposed in this study, Fig. 6b illustrates the integrated modeling strategy of direct catalytic cracking of offshore crude oil using a two-stage riser reactor process. Intuitively, after the first stage of preheating and flash evaporation of offshore crude oil, the light fraction (i.e., naphtha fraction) is sent to the bottom of the second stage riser reactor. After the second stage of preheating and flashing, the heavy fraction is separated into two fractions, namely kerosene and heavy oil. The kerosene fraction is sent to the middle of the second-stage riser reactor. Then, the heavy oil is separated into diesel fraction and heavy oil fraction after the third stage of preheating and flash evaporation. The diesel fraction is sent to the top of the secondary riser reactor. The reason for setting the above partition reaction configuration is the difference in activation energy and cracking difficulty of different fractions. The three feeding points in the No. 2 riser represent different reaction areas, namely the naphtha reaction area, kerosene reaction area, and diesel reaction area. Depending on the degree of reaction, these areas are drawn with different depth colors (the darker the color, the higher the reaction temperature). The reaction temperature of Riser 2# will be higher than that of Riser 1#. In addition, the above configuration can be judged according to the flow direction of the regenerated catalyst. The naphtha reaction area will be arranged near the slide of

the high-temperature regenerated catalyst. The high-temperature regenerated catalyst will be fluidized and directly in contact with the naphtha feed countercurrent. The temperature of this part of the regenerated catalyst can exceed 760 ℃. The kerosene fraction cracking reaction zone is located in the middle of the No. 2 riser, and the top is the diesel reaction zone with a low reaction temperature. In addition, other heavy oil fractions enter the bottom of the No. 1 riser. Therefore, the integrated model of reaction process configuration includes two reactor models and four feed points in a two-stage riser reactor. The advantage of this configuration is that the differential fraction in crude oil can be cracked according to a reasonable reaction degree to achieve directional conversion according to the designed reaction depth. Based on the above analysis, we firmly believe that based on the advantages of regional reaction of a two-stage riser reactor with multi-stage injection, by controlling the reactor temperature in different regions, offshore crude oil can be directionally catalytic cracked to produce olefins and light aromatics.

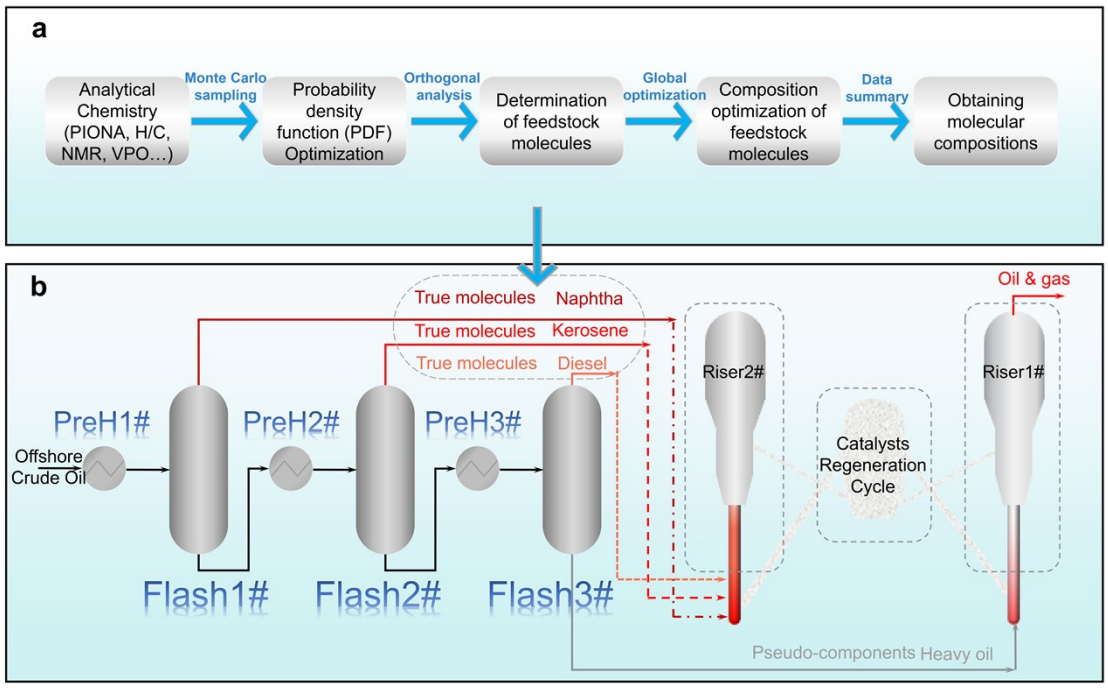

Fig. S1. The novel modeling strategy for direct catalytic cracking of offshore crude oil to chemicals: (a) implementation steps of molecular level reconstruction technology for a light fraction of offshore crude oil; (b) Flow chart of integrated modeling strategy for reaction process of two-stage riser reactor.

In this study, the integral algorithm developed by Aspen HYSYS is used to rebuild the molecules of light petroleum fractions [1], which compresses thousands of

molecules generated by the Monte Carlo sampling algorithm to hundreds [2]. It can ensure that the obtained properties are not much different from the experimental values. In Aspen HYSYS, the detailed molecular reconstruction step is shown as follows. The first input is the analysis data (element composition, molecular weight, boiling point, etc.) from Aspen HYSYS Crude Oil Assay Management. Then, according to the different properties of different groups, the distribution types and parameters of the probability density function of each molecular component are determined. A set of virtual molecular sets is obtained by sampling the distribution function, and its properties are calculated. It will be retained if the gap between the properties and the target analysis meets the requirements. Otherwise, the distribution function will continue to be optimized through the global optimization algorithm until the properties of the target molecular set corresponding to the obtained parameters meet the requirements. Fig. S1 shows the flow of the molecular reconstruction algorithm in Aspen HYSYS.

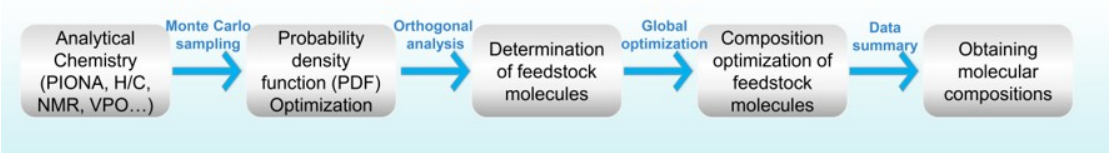

Fig. S1 The flow of the molecular reconstruction algorithm in Aspen HYSYS.

Fig. S2-S4 shows the detailed step screenshots of the molecular reconstruction method adopted in Aspen HYSYS software. Taking the characterization of crude oil as an example, it is necessary to confirm further its different molecular categories in Fig. S2 (including hydrocarbon molecules, sulfur molecules, neutral nitrogen molecules, porphyrin molecules, etc.). Select the **“启用回归”** button (as shown in Fig. S3) and click **“运行评估”** again. Aspen HYSYS crude oil assay management will automatically conduct molecular sampling and reconstruction. The detailed molecular properties of different fractions of crude oil displayed in Aspen HYSYS crude oil assay management after the calculation is shown in Fig. S2-S4.

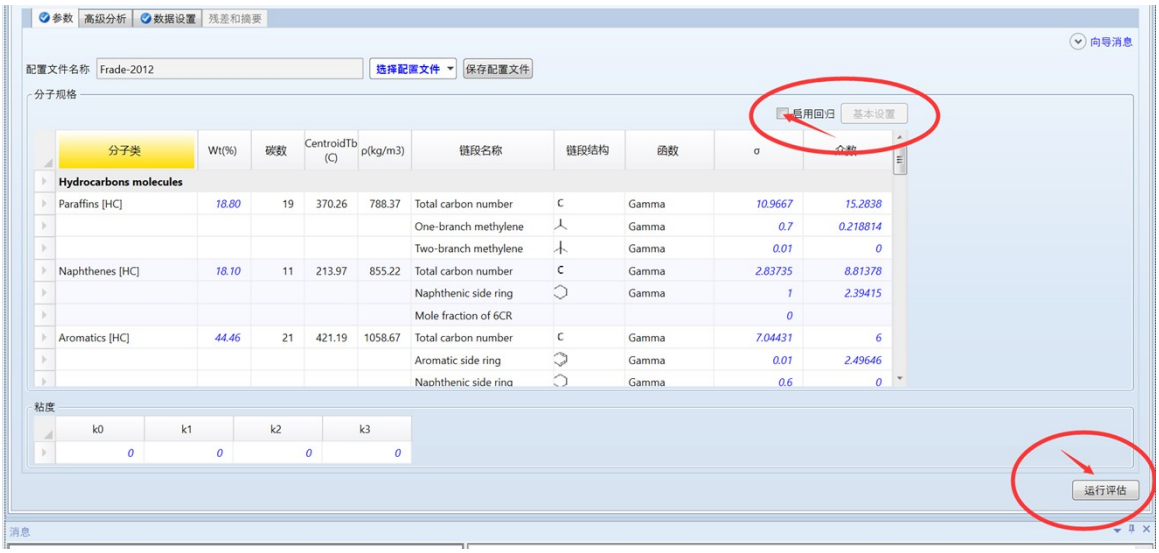

Fig. S2 Molecular reconstruction method: step screenshot of Aspen HYSYS software

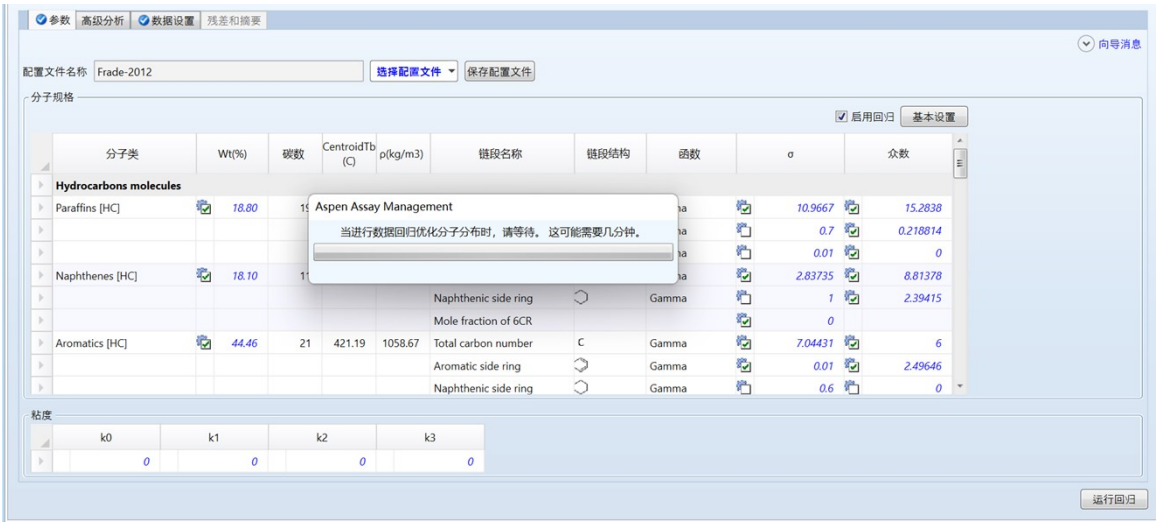

Fig. S3 Run regression calculation

Fig. S4 Molecular reconstruction results: molecular properties of different fractions

The molecular composition reconstruction results of offshore crude oil naphtha fractions (true boiling points: 30℃~160℃) are shown in Fig. S5, and more detailed molecular composition information of naphtha is shown in Table S1.

分子组成
分子物性
分子绘图

	Volume Fraction	Weight Fraction
tr2-Butene	0.0000	0.0000
cis2-Butene	0.0000	0.0000
22DiMePropane	0.0000	0.0000
C5 Iso paraffin with multiple branch	0.0000	0.0000
3MeBut1ene	0.0000	0.0000
C5 Iso paraffin with one branch	0.0000	0.0000
2MeButane	0.0000	0.0000
Pent1ene	0.0000	0.0000
2MeBut1ene	0.0000	0.0000
C5 Normal paraffin	0.0000	0.0000
Pentane	3.558e-002	3.080e-002
C5 Normal olefin	0.0000	0.0000
C5 Iso olefin with one branch	0.0000	0.0000
Pent2ene	0.0000	0.0000
2MeBut2ene	0.0000	0.0000
33DiMeBut1ene	0.0000	0.0000
CPentane	7.344e-004	7.557e-004
C5 Cyclohexane	0.0000	0.0000
22DiMeButane	0.0000	0.0000
3MePent1ene	0.0000	0.0000
4MePent1ene	0.0000	0.0000
23DiMeBut1ene	0.0000	0.0000
4MePent2ene	0.0000	0.0000
C6 Iso paraffin with multiple branch	0.0000	0.0000
23DiMeButane	3.283e-003	3.069e-003
C6 Iso paraffin with one branch	0.0000	0.0000
2MePentane	4.358e-012	3.931e-012
2MePent1ene	0.0000	0.0000
3MePentane	2.791e-002	2.561e-002

Fig. S5 The molecular composition reconstruction results of offshore crude oil naphtha fractions

Table S1. More detailed molecular composition information of offshore crude oil naphtha fractions (30℃-160℃)

No.	Components	Wt%
1	H2	0
2	H2S	0
3	NH3	0
4	Methane	0
5	C1 Light Paraffin	0
6	Ethene	0
7	C2 Light olefin	0
8	Ethane	0

9	C2 Light Paraffin	0
10	C3 Light olefin	0
11	Prop1ene	0
12	C3 Light Paraffin	0
13	Propane	0
14	2MePropane	0
15	2MeProp1ene	0
16	C4 Light olefin	0
17	But1ene	0
18	C4 Light Paraffin	0
19	Butane	0
20	tr2-Butene	0
21	cis2-Butene	0
22	22DiMePropane	0
23	C5 Iso paraffin with multiple branch	0
24	3MeBut1ene	0
25	C5 Iso paraffin with one branch	0
26	2MeButane	0
27	Pent1ene	0
28	2MeBut1ene	0
29	C5 Normal paraffin	0
30	Pentane	3.08E-02
31	C5 Normal olefin	0
32	C5 Iso olefin with one branch	0
33	Pent2ene	0
34	2MeBut2ene	0
35	33DiMeBut1ene	0
36	CPentane	7.56E-04
37	C5 Cyclohexane	0
38	22DiMeButane	0
39	3MePent1ene	0
40	4MePent1ene	0
41	23DiMeBut1ene	0
42	4MePent2ene	0
43	C6 Iso paraffin with multiple branch	0
44	23DiMeButane	3.07E-03
45	C6 Iso paraffin with one branch	0
46	2MePentane	3.93E-12

47	2MePent1ene	0
48	3MePentane	2.56E-02
49	Hex1ene	0
50	2EtBut1ene	0
51	C6 Iso olefin with multiple branch	0
52	C6 Normal olefin	0
53	Hex3ene	0
54	2MePent2ene	0
55	3MePent2ene	0
56	Hex2ene	0
57	Hexane	4.00E-02
58	C6 Normal paraffin	0
59	C6 Iso olefin with one branch	0
60	MeCPentane	1.65E-03
61	23DiMeBut2ene	0
62	C7 Iso paraffin with multiple branch	1.79E-03
63	22DiMePentane	0
64	Benzene	8.09E-04
65	C6 Benzene	0
66	24DiMePentane	7.38E-14
67	C6 Cyclohexane	0
68	CHexane	0
69	223TrMeButane	0
70	C7 Iso olefin with multiple branch	0
71	C4 Thiophene	6.22E-07
72	33DiMePentane	0
73	C4 Tetrahydropyrrole	0
74	11DiMeCPentane	5.70E-14
75	23DiMePentane	1.30E-02
76	C7 Iso olefin with one branch	0
77	C7 Iso paraffin with one branch	1.79E-03
78	2MeHexane	3.11E-13
79	3MeHexane	5.92E-02
80	13DiMeCPentane	7.31E-03
81	3EtPentane	2.03E-03
82	C7 Normal olefin	0
83	C4 Sulfide/mercaptan	7.57E-09

84	Heptane	4.78E-02
85	C7 Normal paraffin	1.79E-03
86	224TrMePentane	0
87	12DiMeCPentane	1.37E-03
88	H2O	0
89	MeCHexane	0
90	C7 Cyclohexane	1.19E-02
91	EtCPentane	3.71E-04
92	113TrMetCPentane	8.17E-14
93	C5 Tetrahydropyrrole	0
94	C8 Iso paraffin with multiple branch	3.19E-03
95	22DiMeHexane	0
96	C8 Iso olefin with multiple branch	0
97	124TrMetCPentane	7.30E-06
98	25DiMeHexane	7.87E-14
99	223TrMePentane	0
100	24DiMeHexane	1.16E-02
101	Toluene	1.07E-03
102	C7 Benzene	0
103	33DiMeHexane	0
104	C5 Thiophene	1.43E-06
105	234TrMePentane	9.91E-04
106	1Me3EtCPentane	3.74E-03
107	112TrMetCPentane	6.53E-03
108	233TrMePentane	0
109	C5 Pyrridine	0
110	23DiMeHexane	5.41E-03
111	2Me3EtPentane	1.89E-03
112	C8 Iso olefin with one branch	0
113	123TrMetCPentane	1.11E-02
114	2MeHeptane	2.53E-02
115	C8 Iso paraffin with one branch	3.19E-03
116	4MeHeptane	4.45E-02
117	34DiMeHexane	5.13E-04
118	3MeHeptane	2.26E-03
119	3Me3EtPentane	0
120	3EtHexane	1.42E-02
121	11DiMeCHexane	0
122	1Me1EtCPentane	3.79E-03

123	C4 Tetrahydrothiophene	4.12E-08
124	14DiMeCHexane	0
125	13DiMeCHexane	0
126	IsoPrCPentane	1.27E-03
127	C8 Normal olefin	0
128	1124TeMeCPentane	1.05E-05
129	225TrMeHexane	0
130	12DiMeCHexane	0
131	Octane	5.39E-02
132	C8 Normal paraffin	3.19E-03
133	1Me2EtPentane	4.77E-03
134	224TrMeHexane	0
135	C5 Sulfide/mercaptan	8.60E-09
136	11DiMe3EtCPentane	3.15E-04
137	13DiMe1EtCPentane	1.72E-03
138	1123TeMeCPentane	4.65E-03
139	C4 Pyrrole	0
140	C9 Iso olefin with multiple branch	0
141	244TrMeHexane	0
142	235TrMeHexane	2.37E-14
143	C6 Tetrahydropyrrole	0
144	PrCPentane	5.33E-04
145	C8 Cyclohexane	6.85E-02
146	EtCHexane	0
147	1125TeMeCPentane	8.60E-03
148	24DiMeHeptane	1.53E-03
149	22DiMeHeptane	0
150	223TrMeHexane	0
151	2Me4EtHeptane	9.54E-03
152	1Me1IsoPrCPentane	1.34E-13
153	25DiMeHeptane	1.68E-02
154	C6 Thiophene	4.01E-06
155	44DiMeHeptane	0
156	114TrMeCHexane	0
157	1122TeMeCPentane	1.25E-02
158	26DiMeHeptane	7.80E-03
159	35DiMeHeptane	5.40E-03
160	EtBenzene	2.69E-14
161	C8 Benzene	0
162	C9 Iso paraffin with multiple branch	6.40E-03
163	24DiMe1EtCPentane	1.53E-02

164	N5_1_C9	0
165	113TrMeCHexane	0
166	33DiMeHeptane	0
167	11DiMe2EtCPentane	1.66E-02
168	12DiMe1EtCPentane	1.64E-02
169	233TrMeHexane	0
170	2Me3EtHeptane	3.21E-03
171	PXylene	1.97E-03
172	C5 Tetrahydrothiophene	9.40E-08
173	234TrMeHexane	1.55E-04
174	MXylene	3.46E-03
175	334TrMeHexane	0
176	1Me13IsoPrCPentane	5.29E-03
177	13DiMe2EtCPentane	1.31E-02
178	12DiMe3EtCPentane	1.51E-02
179	13DiEtCPentane	6.52E-03
180	1Me3PrCPentane	8.54E-03
181	4Me3EtHeptane	1.89E-03
182	3Me3EtHeptane	0
183	34DiMeHeptane	1.05E-03
184	135TrMeCHexane	0
185	23DiMeHeptane	5.11E-04
186	C9 Iso olefin with one branch	0
187	4EtHeptane	3.53E-13
188	124TrMeCHexane	0
189	1Me2IsoPrCPentane	1.89E-02
190	3EtHeptane	4.30E-02
191	2MeOctane	4.53E-02
192	C9 Iso paraffin with one branch	3.35E-03
193	3MeOctane	3.28E-02
194	C6 Pyrridine	0
195	OXylene	1.10E-03
196	4MeOctane	8.85E-03
197	1IsoButCPentane	1.23E-02
198	112TrMeCHexane	0
199	C9 Normal olefin	1.76E-04
200	1Me2PrCPentane	4.83E-03
201	12DiEtCPentane	3.49E-03
202	C6 Tetrahydrothiophene	1.05E-07
203	C5 Pyrrole	0
204	3Me1EtCHexane	0

205	1Me1PrCPentane	1.70E-03
206	11DiEtCPentane	1.15E-03
207	2SecBuCPentane	3.96E-03
208	4Me1EtCHexane	0
209	1SecBuCPentane	8.73E-04
210	Nonane	5.79E-02
211	C9 Normal paraffin	3.35E-03
212	123TrMeCHexane	0
213	2Me1EtCHexane	0
214	1Me1EtCHexane	0
215	IsoPrBenzene	1.63E-03
216	C6 Sulfide/mercaptan	1.28E-08
217	IsoPrCHexane	0
218	C7 Tetrahydropyrrole	0
219	C10 Iso olefin with multiple branch	0
220	BuCPentane	7.68E-04
221	PrCHexane	0
222	C9 Cyclohexane	0
223	C10 Iso paraffin with multiple branch	4.56E-02
224	C7 Thiophene	2.66E-06
225	PrBenzene	2.18E-03
226	C9 Benzene	0
227	4Me1EtBenzene	2.44E-09
228	3Me1EtBenzene	2.40E-09
229	N5_1_C10	0
230	135TrmeBenzene	1.50E-09
231	2Me1EtBenzene	7.34E-10
232	C10 Iso olefin with one branch	0
233	C10 Iso paraffin with one branch	7.02E-08
234	C7 Pyrridine	0
235	124TrmeBenzene	3.23E-10
	Total	**1**

Naming rules and examples shown in the Table S1: 2MePropane: 2-MethylPropane; 23DiMeButane: 2,3-DimethylButane; 112TrMeCHexane: 1,1,2-TrimethylCyclohexane; 11DiEtCPentane 1,1-DiEthylCyclopentane; 1Me2PrCPentane: 1-methy,2propyl, Cyclopentane; C11 Normal paraffin: Undecane; C11 Iso paraffin with one branch: Isoundecane

In addition, to verify the accuracy of the molecular reconstruction method proposed in

this study, we compared and verified the distillation curve and density of naphtha before and after molecular reconstruction. These results are shown in Table S2. It can be seen from the table that the relative error between the naphtha distillation curve and density before and after molecular reconstruction is less than 5.0%. The above results verify the accuracy of the molecular property reconstruction of naphtha proposed by us.

Table S2. Comparison results of naphtha before and after reconstruction

Items	Naphtha before molecular reconstruction	Naphtha after molecular reconstruction	relative errors %
Initial boiling point/℃	36.06	34.56	4.16
10%/℃	68.40	65.24	4.62
30%/℃	111.38	116.36	4.47
50%/℃	131.0	134.22	2.46
70%/℃	140.2	139.63	0.41
90%/℃	150.8	153.57	1.84
Final boiling point/℃	160.00	162.52	1.58
Density (kg/m^3)	721.5	724.4	0.40

The figure of comparison results of naphtha before and after reconstruction is shown in Figure S6.

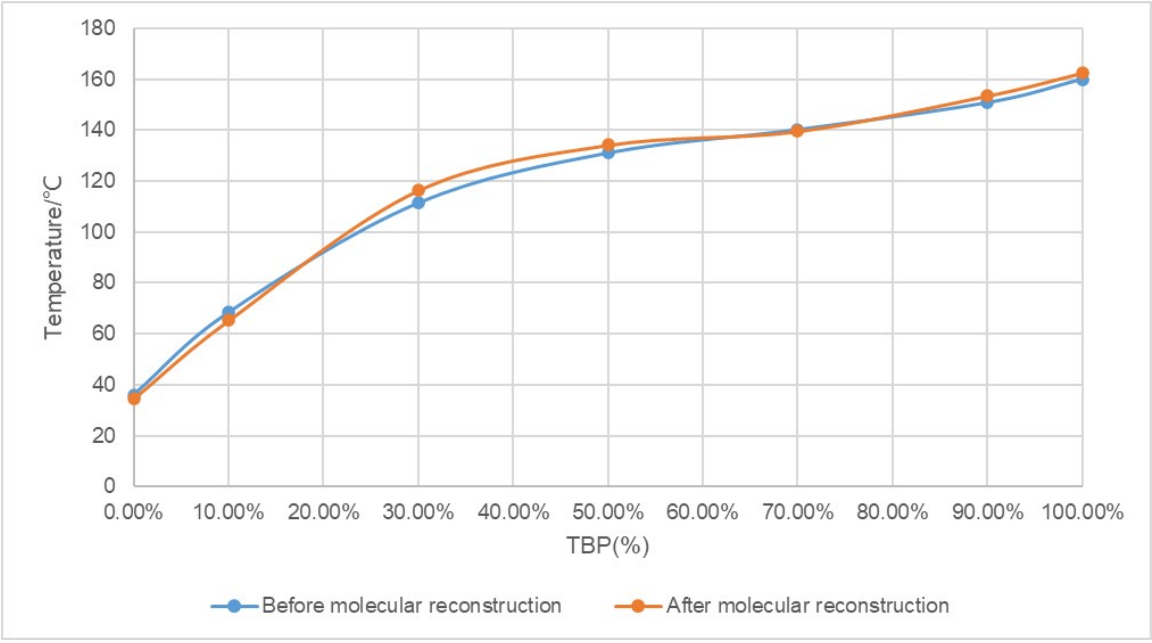

Fig. S6. Comparison results of naphtha before and after reconstruction

The molecular composition reconstruction results of offshore crude oil kerosene fractions (true boiling points: 160℃~210℃) are shown in Fig. S7, and more detailed molecular composition information of kerosene is shown in Table S3.


分子组成
分子物性
分子绘图

	Volume Fraction	Weight Fraction	Mole Fraction
Nonane	8.541e-002	8.051e-002	9.167e-002
C9 Normal paraffin	4.944e-003	4.660e-003	5.307e-003
123TrMeCHexane	0.0000	0.0000	0.0000
2Me1EtCHexane	0.0000	0.0000	0.0000
1Me1EtCHexane	0.0000	0.0000	0.0000
IsoPrBenzene	2.006e-003	2.270e-003	2.757e-003
C6 Sulfide/mercaptan	1.607e-008	1.777e-008	2.195e-008
IsoPrCHexane	0.0000	0.0000	0.0000
C7 Tetrahydropyrrole	0.0000	0.0000	0.0000
C10 Iso olefin with multiple branch	0.0000	0.0000	0.0000
BuCPentane	1.036e-003	1.067e-003	1.234e-003
PrCHexane	0.0000	0.0000	0.0000
C9 Cyclohexane	0.0000	0.0000	0.0000
C10 Iso paraffin with multiple branch	6.577e-002	6.332e-002	6.499e-002
C7 Thiophene	2.909e-006	3.696e-006	4.276e-006
PrBenzene	2.675e-003	3.026e-003	3.675e-003
C9 Benzene	0.0000	0.0000	0.0000
4Me1EtBenzene	5.546e-003	6.266e-003	7.611e-003
3Me1EtBenzene	5.445e-003	6.186e-003	7.514e-003
N5_1_C10	0.0000	0.0000	0.0000
135TrmeBenzene	3.401e-003	3.861e-003	4.690e-003
2Me1EtBenzene	1.635e-003	1.889e-003	2.295e-003
C10 Iso olefin with one branch	0.0000	0.0000	0.0000
C10 Iso paraffin with one branch	0.1869	0.1808	0.1855
C7 Pyrridine	0.0000	0.0000	0.0000
124TrmeBenzene	7.228e-004	8.309e-004	1.009e-003
C10 Normal olefin	0.0000	0.0000	0.0000
C10 Cyclohexane	0.0000	0.0000	0.0000

Fig. S7 The molecular composition reconstruction results of offshore crude oil kerosene fractions

Table S3. More detailed molecular composition information of kerosene

No.	Components	Wt%
1	Nonane	8.05E-02
2	C9 Normal paraffin	4.66E-03
3	123TrMeCHexane	0
4	2Me1EtCHexane	0
5	1Me1EtCHexane	0
6	IsoPrBenzene	2.27E-03
7	C6 Sulfide/mercaptan	1.78E-08
8	IsoPrCHexane	0
9	C7 Tetrahydropyrrole	0
10	C10 Iso olefin with multiple branch	0
11	BuCPentane	1.07E-03
12	PrCHexane	0
13	C9 Cyclohexane	0

14	C10 Iso paraffin with multiple branch	6.33E-02
15	C7 Thiophene	3.70E-06
16	PrBenzene	3.03E-03
17	C9 Benzene	0
18	4Me1EtBenzene	6.27E-03
19	3Me1EtBenzene	6.19E-03
20	N5_1_C10	0
21	135TrmeBenzene	3.86E-03
22	2Me1EtBenzene	1.89E-03
23	C10 Iso olefin with one branch	0
24	C10 Iso paraffin with one branch	0.180758
25	C7 Pyrridine	0
26	124TrmeBenzene	8.31E-04
27	C10 Normal olefin	0
28	C10 Cyclohexane	0
29	C7 Tetrahydrothiophene	2.68E-07
30	C8 Thiophene	4.48E-06
31	C10 Normal paraffin	9.52E-02
32	123TrmeBenzene	3.00E-04
33	C11 Iso paraffin with multiple branch	2.21E-02
34	C7 Sulfide/mercaptan	1.63E-08
35	C9 Indane	6.57E-04
36	C8 Tetrahydropyrrole	0
37	N5_1_C11	0
38	C10 Benzene	6.84E-02
39	C11 Iso olefin with one branch	0
40	C11 Iso olefin with multiple branch	0
41	C10 Decalin	2.66E-02
42	C11 Iso paraffin with one branch	0.154152
43	C8 Pyrridine	0
44	C9 Indene	0
45	C12 Iso olefin with multiple branch	0
46	C11 Normal olefin	0
47	C8 Tetrahydrothiophene	3.88E-07
48	C11 Normal paraffin	9.79E-02

49	C11 Cyclohexane	0
50	C7 Pyrrole	0
51	C8 Sulfide/mercaptan	1.77E-08
52	C8 Octahydrobenzothiophene	6.47E-08
53	C9 Thiophene	4.84E-06
54	C9 Tetrahydropyrrole	0
55	C12 Iso paraffin with multiple branch	5.41E-03
56	C8 Octahydroindole	0
57	C11 Benzene	4.46E-02
58	C12 Iso olefin with one branch	0
59	C10 Tetralin	2.89E-03
60	N5_1_C12	0
61	C11 Decalin	3.33E-02
62	C12 Iso paraffin with one branch	9.38E-02
63	C10 Indane	5.95E-10
64	C9 Octahydrobenzothiophene	8.38E-14
65	C9 Tetrahydrothiophene	2.51E-13
66	C12 Normal olefin	0
67	C9 Octahydroindole	1.25E-10
68	C10 Indene	0
69	C12 Normal paraffin	5.84E-08
70	C9 Pyrridine	0
71	C8 Dihydrobenzothiophene	8.12E-22
72	C10 Naphthalene	0
73	C13 Iso paraffin with one branch	3.72E-08
74	C11 Indane	1.08E-09
75	C8 Pyrrole	0
76	C12 Cyclohexane	0
77	C10 Thiophene	2.07E-12
78	C9 Sulfide/mercaptan	3.80E-15
	Total	1.00

We also compared and validated kerosene's distillation curves and densities before and after molecular reconstruction. These results are shown in Table S4. As can be seen from the table, the relative error between the distillation curve and the kerosene density

before and after molecular reconstruction is less than 2%. The accuracy of the molecular remodeling characteristics of kerosene can be further verified.

Table S4. Comparison results of kerosene before and after reconstruction

Items	Kerosene before molecular reconstruction	Kerosene after molecular reconstruction	relative errors
Initial boiling point/℃	150.82	153.56	1.82
10%/℃	156.84	158.45	1.03
30%/℃	166.36	164.32	1.22
50%/℃	180.56	178.42	1.18
70%/℃	188.29	191.44	1.67
90%/℃	204.16	203.21	0.47
Final boiling point/℃	210.00	210.00	0.00
Density (kg/m^3)	758.30	754.24	0.54

The figure of comparison results of kerosene before and after reconstruction is shown in Figure S8.

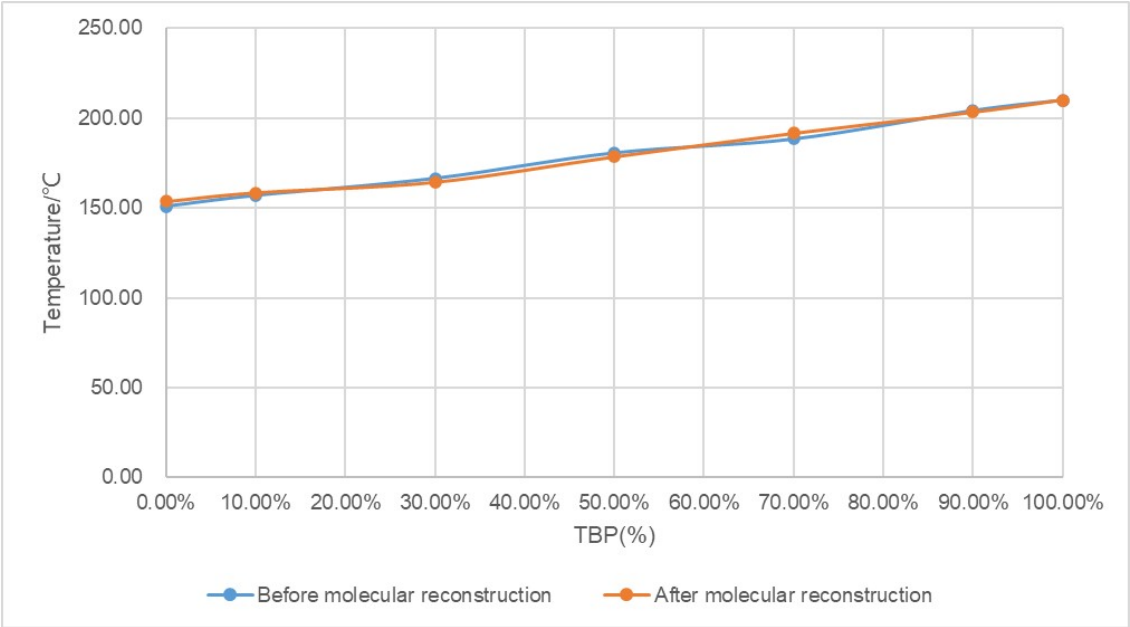

Fig. S8. Comparison results of kerosene before and after reconstruction

The molecular composition reconstruction results of diesel fractions (true boiling points: 211℃~260℃) are shown in Fig. S9, and more detailed molecular composition information of diesel is shown in Table S5.

分子组成
分子物性
分子绘图

	Volume Fraction	Weight Fraction	Mole Fraction
C12 Iso paraffin with multiple branch	5.420e-003	5.048e-003	5.288e-003
C8 Octahydroindole	0.0000	0.0000	0.0000
C11 Benzene	3.814e-002	4.164e-002	5.011e-002
C12 Iso olefin with one branch	0.0000	0.0000	0.0000
C10 Tetralin	2.195e-003	2.700e-003	3.643e-003
N5_1_C12	0.0000	0.0000	0.0000
C11 Decalin	2.859e-002	3.114e-002	3.649e-002
C12 Iso paraffin with one branch	9.320e-002	8.758e-002	9.175e-002
C10 Indane	8.646e-004	1.028e-003	1.387e-003
C9 Octahydrobenzothiophene	1.057e-007	1.449e-007	1.654e-007
C9 Tetrahydrothiophene	3.728e-007	4.340e-007	4.892e-007
C12 Normal olefin	0.0000	0.0000	0.0000
C9 Octahydroindole	1.923e-004	2.159e-004	2.766e-004
C10 Indene	0.0000	0.0000	0.0000
C12 Normal paraffin	0.1076	0.1010	0.1058
C9 Pyrridine	0.0000	0.0000	0.0000
C8 Dihydrobenzothiophene	9.670e-016	1.404e-015	1.839e-015
C10 Naphthalene	0.0000	0.0000	0.0000
C13 Iso paraffin with one branch	6.786e-002	6.431e-002	6.224e-002
C11 Indane	1.578e-003	1.871e-003	2.282e-003
C8 Pyrrole	0.0000	0.0000	0.0000
C12 Cyclohexane	0.0000	0.0000	0.0000
C10 Thiophene	2.975e-006	3.582e-006	3.797e-006
C9 Sulfide/mercaptan	6.217e-009	6.575e-009	7.318e-009
C10 Tetrahydropyrrole	0.0000	0.0000	0.0000
C12 Benzene	4.800e-002	5.235e-002	5.755e-002
C13 Iso paraffin with multiple branch	5.740e-003	5.404e-003	5.231e-003
C8 Benzothiophene	6.023e-006	9.149e-006	1.216e-005
C11 Tetralin	3.087e-003	3.711e-003	4.527e-003
C9 Tetrahydroquinoline	0.0000	0.0000	0.0000

Fig. S9 The molecular composition reconstruction results of offshore crude oil diesel fractions

Table S5. More detailed molecular composition information of offshore crude oil diesel

No.	Components	Wt%
1	C12 Iso paraffin with multiple branch	5.05E-03
2	C8 Octahydroindole	0
3	C11 Benzene	4.16E-02
4	C12 Iso olefin with one branch	0
5	C10 Tetralin	2.70E-03
6	N5_1_C12	0
7	C11 Decalin	3.11E-02
8	C12 Iso paraffin with one branch	8.76E-02
9	C10 Indane	1.03E-03
10	C9 Octahydrobenzothiophene	1.45E-07
11	C9 Tetrahydrothiophene	4.34E-07
12	C12 Normal olefin	0
13	C9 Octahydroindole	2.16E-04

14	C10 Indene	0
15	C12 Normal paraffin	0.101018
16	C9 Pyrridine	0
17	C8 Dihydrobenzothiophene	1.40E-15
18	C10 Naphthalene	0
19	C13 Iso paraffin with one branch	6.43E-02
20	C11 Indane	1.87E-03
21	C8 Pyrrole	0
22	C12 Cyclohexane	0
23	C10 Thiophene	3.58E-06
24	C9 Sulfide/mercaptan	6.57E-09
25	C10 Tetrahydropyrrole	0
26	C12 Benzene	5.23E-02
27	C13 Iso paraffin with multiple branch	5.40E-03
28	C8 Benzothiophene	9.15E-06
29	C11 Tetralin	3.71E-03
30	C9 Tetrahydroquinoline	0
31	C13 Iso olefin with one branch	0
32	C13 Iso olefin with multiple branch	0
33	C12 Decalin	4.10E-02
34	C9 Dihydrobenzothiophene	1.10E-16
35	C10 Octahydroindole	0
36	C13 Normal olefin	0
37	C13 Normal paraffin	9.73E-02
38	C10 Pyrridine	0
39	C9 Quinolone	0
40	C10 Tetrahydrothiophene	4.64E-07
41	C11 Indene	0
42	C9 Pyrrole	0
43	C11 Tetrahydropyrrole	0
44	C14 Iso paraffin with multiple branch	5.12E-03
45	C13 Cyclohexane	9.87E-02
46	C12 Indane	3.54E-03
47	C10 Sulfide/mercaptan	2.10E-08
48	C9 Benzothiophene	1.48E-05
49	C11 Thiophene	3.81E-06
50	C14 Iso paraffin with one branch	3.30E-02

51	C12 Tetralin	6.80E-04
52	C11 Naphthalene	0
53	C10 Tetrahydroquinoline	0
54	C14 Iso olefin with multiple branch	0
55	C14 Iso olefin with one branch	0
56	C13 Decalin	6.21E-02
57	C11 Octahydroindole	0
58	C10 Octahydrobenzothiophene	1.55E-07
59	C10 Dihydrobenzothiophene	1.63E-15
60	C14 Normal olefin	0
61	C13 Benzene	1.79E-02
62	C8 Indole	0
63	C14 Normal paraffin	9.22E-02
64	C11 Pyrridine	0
65	C11 Tetrahydrothiophene	4.92E-07
66	C14 Bicyclohexyl	3.39E-02
67	C10 Pyrrole	0
68	C15 Iso paraffin with multiple branch	4.77E-03
69	C12 Tetrahydropyrrole	0
70	C12 Indene	0
71	C14 Cyclohexane	0.107711
72	C11 Sulfide/mercaptan	2.23E-08
73	C13 Indane	3.94E-03
74	C11 Tetrahydroquinoline	0
75	C10 Benzothiophene	1.06E-05
	Total	**1.00E+00**

We also compared and verified diesel's distillation curve and density before and after molecular reconstruction. These results are shown in Table S6. It can be seen from Table S6 that the relative error between the distillation curve and the density of diesel before and after molecular reconstruction is less than 2.5%. The accuracy of the reconstructed properties of diesel molecules can be further verified.

Table S6. Comparison results of offshore crude oil in diesel fractions before and after reconstruction

Items	Diesel before molecular	Diesel after molecular reconstruction	relative errors%

	reconstruction		
Initial boiling point/℃	200.60	204.65	2.02
10%/℃	206.76	209.34	1.25
30%/℃	216.71	211.45	2.43
50%/℃	233.19	237.29	1.76
70%/℃	245.43	241.10	1.76
90%/℃	256.12	257.42	0.51
Final boiling point/℃	260.00	260.00	0.00
Density (kg/m_3)	794.68	798.32	0.46

The figure of comparison results of diesel before and after reconstruction is shown in Figure S10.

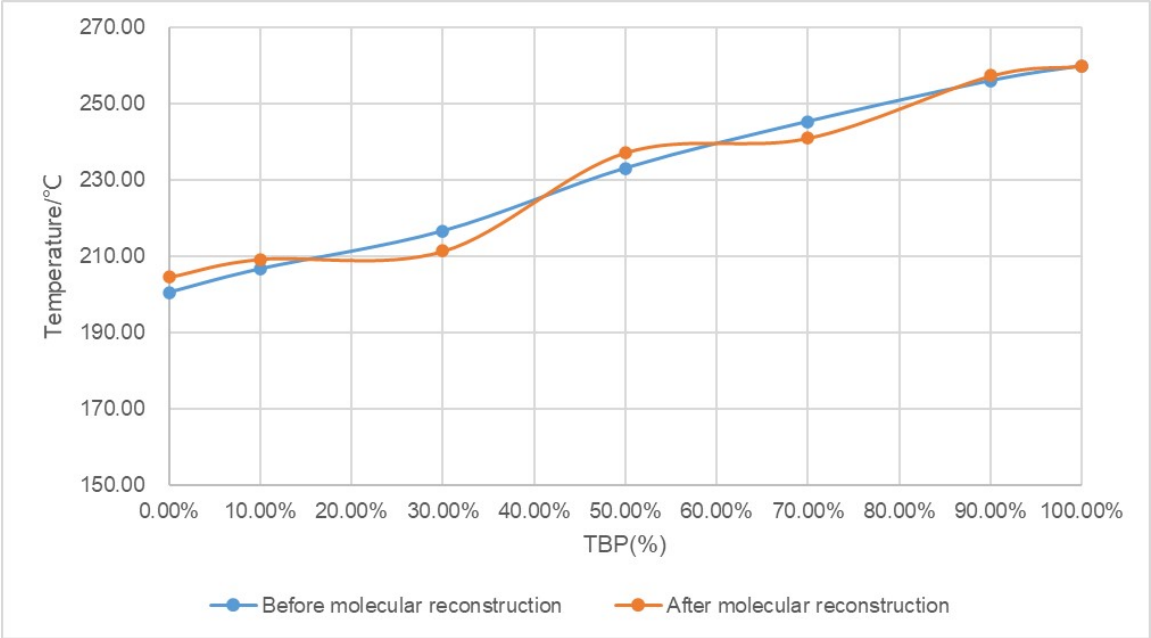

Fig. S10 The molecular composition reconstruction results of offshore crude oil diesel fractions

Comparison results of Naphtha+kerosone+diesel results are shown in Table S7.

Table S7. Comparison results of Naphtha+kerosone+diesel fractions in offshore crude oil.

No.	Components	Wt%
1	H2	0
2	H2S	0
3	NH3	0
4	Methane	0
5	C1 Light Paraffin	0
6	Ethene	0
7	C2 Light olefin	0

8	Ethane	0
9	C2 Light Paraffin	0
10	C3 Light olefin	0
11	Prop1ene	0
12	C3 Light Paraffin	0
13	Propane	0
14	2MePropane	0
15	2MeProp1ene	0
16	C4 Light olefin	0
17	But1ene	0
18	C4 Light Paraffin	0
19	Butane	0
20	tr2-Butene	0
21	cis2-Butene	0
22	22DiMePropane	0
23	C5 Iso paraffin with multiple branch	0
24	3MeBut1ene	0
25	C5 Iso paraffin with one branch	0
26	2MeButane	0
27	Pent1ene	0
28	2MeBut1ene	0
29	C5 Normal paraffin	0
30	Pentane	1.49E-02
31	C5 Normal olefin	0
32	C5 Iso olefin with one branch	0
33	Pent2ene	0
34	2MeBut2ene	0
35	33DiMeBut1ene	0
36	CPentane	3.66E-04
37	C5 Cyclohexane	0
38	22DiMeButane	0
39	3MePent1ene	0
40	4MePent1ene	0
41	23DiMeBut1ene	0
42	4MePent2ene	0
43	C6 Iso paraffin with multiple branch	0
44	23DiMeButane	1.49E-03
45	C6 Iso paraffin with one branch	0
46	2MePentane	1.90E-12
47	2MePent1ene	0
48	3MePentane	1.24E-02

49	Hex1ene	0
50	2EtBut1ene	0
51	C6 Iso olefin with multiple branch	0
52	C6 Normal olefin	0
53	Hex3ene	0
54	2MePent2ene	0
55	3MePent2ene	0
56	Hex2ene	0
57	Hexane	1.93E-02
58	C6 Normal paraffin	0
59	C6 Iso olefin with one branch	0
60	MeCPentane	7.96E-04
61	23DiMeBut2ene	0
62	C7 Iso paraffin with multiple branch	8.68E-04
63	22DiMePentane	0
64	Benzene	3.92E-04
65	C6 Benzene	0
66	24DiMePentane	3.57E-14
67	C6 Cyclohexane	0
68	CHexane	0
69	223TrMeButane	0
70	C7 Iso olefin with multiple branch	0
71	C4 Thiophene	3.01E-07
72	33DiMePentane	0
73	C4 Tetrahydropyrrole	0
74	11DiMeCPentane	2.76E-14
75	23DiMePentane	6.28E-03
76	C7 Iso olefin with one branch	0
77	C7 Iso paraffin with one branch	8.68E-04
78	2MeHexane	1.50E-13
79	3MeHexane	2.87E-02
80	13DiMeCPentane	3.54E-03
81	3EtPentane	9.81E-04
82	C7 Normal olefin	0
83	C4 Sulfide/mercaptan	3.66E-09
84	Heptane	2.31E-02
85	C7 Normal paraffin	8.68E-04
86	224TrMePentane	0
87	12DiMeCPentane	6.63E-04
88	H2O	0

89	MeCHexane	0
90	C7 Cyclohexane	5.76E-03
91	EtCPentane	1.80E-04
92	113TrMetCPentane	3.96E-14
93	C5 Tetrahydropyrrole	0
94	C8 Iso paraffin with multiple branch	1.54E-03
95	22DiMeHexane	0
96	C8 Iso olefin with multiple branch	0
97	124TrMetCPentane	3.53E-06
98	25DiMeHexane	3.81E-14
99	223TrMePentane	0
100	24DiMeHexane	5.59E-03
101	Toluene	5.17E-04
102	C7 Benzene	0
103	33DiMeHexane	0
104	C5 Thiophene	6.91E-07
105	234TrMePentane	4.79E-04
106	1Me3EtCPentane	1.81E-03
107	112TrMetCPentane	3.16E-03
108	233TrMePentane	0
109	C5 Pyrridine	0
110	23DiMeHexane	2.62E-03
111	2Me3EtPentane	9.15E-04
112	C8 Iso olefin with one branch	0
113	123TrMetCPentane	5.38E-03
114	2MeHeptane	1.22E-02
115	C8 Iso paraffin with one branch	1.54E-03
116	4MeHeptane	2.15E-02
117	34DiMeHexane	2.48E-04
118	3MeHeptane	1.09E-03
119	3Me3EtPentane	0
120	3EtHexane	6.88E-03
121	11DiMeCHexane	0
122	1Me1EtCPentane	1.83E-03
123	C4 Tetrahydrothiophene	1.99E-08
124	14DiMeCHexane	0
125	13DiMeCHexane	0
126	IsoPrCPentane	6.14E-04
127	C8 Normal olefin	0
128	1124TeMeCPentane	5.09E-06
129	225TrMeHexane	0

130	12DiMeCHexane	0
131	Octane	2.61E-02
132	C8 Normal paraffin	1.54E-03
133	1Me2EtPentane	2.31E-03
134	224TrMeHexane	0
135	C5 Sulfide/mercaptan	4.16E-09
136	11DiMe3EtCPentane	1.53E-04
137	13DiMe1EtCPentane	8.31E-04
138	1123TeMeCPentane	2.25E-03
139	C4 Pyrrole	0
140	C9 Iso olefin with multiple branch	0
141	244TrMeHexane	0
142	235TrMeHexane	1.15E-14
143	C6 Tetrahydropyrrole	0
144	PrCPentane	2.58E-04
145	C8 Cyclohexane	3.31E-02
146	EtCHexane	0
147	1125TeMeCPentane	4.16E-03
148	24DiMeHeptane	7.40E-04
149	22DiMeHeptane	0
150	223TrMeHexane	0
151	2Me4EtHeptane	4.62E-03
152	1Me1IsoPrCPentane	6.48E-14
153	25DiMeHeptane	8.15E-03
154	C6 Thiophene	1.94E-06
155	44DiMeHeptane	0
156	114TrMeCHexane	0
157	1122TeMeCPentane	6.03E-03
158	26DiMeHeptane	3.77E-03
159	35DiMeHeptane	2.61E-03
160	EtBenzene	1.30E-14
161	C8 Benzene	0
162	C9 Iso paraffin with multiple branch	3.10E-03
163	24DiMe1EtCPentane	7.40E-03
164	N5_1_C9	0
165	113TrMeCHexane	0
166	33DiMeHeptane	0
167	11DiMe2EtCPentane	8.04E-03
168	12DiMe1EtCPentane	7.96E-03
169	233TrMeHexane	0
170	2Me3EtHeptane	1.56E-03

171	PXylene	9.51E-04
172	C5 Tetrahydrothiophene	4.55E-08
173	234TrMeHexane	7.48E-05
174	MXylene	1.67E-03
175	334TrMeHexane	0
176	1Me13IsoPrCPentane	2.56E-03
177	13DiMe2EtCPentane	6.33E-03
178	12DiMe3EtCPentane	7.31E-03
179	13DiEtCPentane	3.15E-03
180	1Me3PrCPentane	4.13E-03
181	4Me3EtHeptane	9.13E-04
182	3Me3EtHeptane	0
183	34DiMeHeptane	5.06E-04
184	135TrMeCHexane	0
185	23DiMeHeptane	2.47E-04
186	C9 Iso olefin with one branch	0
187	4EtHeptane	1.71E-13
188	124TrMeCHexane	0
189	1Me2IsoPrCPentane	9.15E-03
190	3EtHeptane	2.08E-02
191	2MeOctane	2.19E-02
192	C9 Iso paraffin with one branch	1.62E-03
193	3MeOctane	1.59E-02
194	C6 Pyrridine	0
195	OXylene	5.34E-04
196	4MeOctane	4.28E-03
197	1IsoButCPentane	5.94E-03
198	112TrMeCHexane	0
199	C9 Normal olefin	8.50E-05
200	1Me2PrCPentane	2.34E-03
201	12DiEtCPentane	1.69E-03
202	C6 Tetrahydrothiophene	5.08E-08
203	C5 Pyrrole	0
204	3Me1EtCHexane	0
205	1Me1PrCPentane	8.21E-04
206	11DiEtCPentane	5.57E-04
207	2SecBuCPentane	1.92E-03
208	4Me1EtCHexane	0
209	1SecBuCPentane	4.23E-04
210	Nonane	2.80E-02
211	C9 Normal paraffin	1.62E-03
212	123TrMeCHexane	0
213	2Me1EtCHexane	0

214	1Me1EtCHexane	0
215	IsoPrBenzene	7.90E-04
216	C6 Sulfide/mercaptan	6.19E-09
217	IsoPrCHexane	0
218	C7 Tetrahydropyrrole	0
219	C10 Iso olefin with multiple branch	0
220	BuCPentane	3.72E-04
221	PrCHexane	0
222	C9 Cyclohexane	0
223	C10 Iso paraffin with multiple branch	2.20E-02
224	C7 Thiophene	1.29E-06
225	PrBenzene	1.05E-03
226	C9 Benzene	0
227	4Me1EtBenzene	1.96E-03
228	3Me1EtBenzene	1.94E-03
229	N5_1_C10	0
230	135TrmeBenzene	1.21E-03
231	2Me1EtBenzene	5.92E-04
232	C10 Iso olefin with one branch	0
233	C10 Iso paraffin with one branch	5.66E-02
234	C7 Pyrridine	0
235	124TrmeBenzene	2.60E-04
236	C10 Normal olefin	0
237	C10 Cyclohexane	0
238	C7 Tetrahydrothiophene	8.39E-08
239	C8 Thiophene	1.40E-06
240	C10 Normal paraffin	2.98E-02
241	123TrmeBenzene	9.41E-05
242	C11 Iso paraffin with multiple branch	6.93E-03
243	C7 Sulfide/mercaptan	5.10E-09
244	C9 Indane	2.06E-04
245	C8 Tetrahydropyrrole	0
246	N5_1_C11	0
247	C10 Benzene	2.14E-02
248	C11 Iso olefin with one branch	0
249	C11 Iso olefin with multiple branch	0
250	C10 Decalin	8.35E-03
251	C11 Iso paraffin with one	4.83E-02

	branch	
252	C8 Pyrridine	0
253	C9 Indene	0
254	C12 Iso olefin with multiple branch	0
255	C11 Normal olefin	0
256	C8 Tetrahydrothiophene	1.22E-07
257	C11 Normal paraffin	3.07E-02
258	C11 Cyclohexane	0
259	C7 Pyrrole	0
260	C8 Sulfide/mercaptan	5.54E-09
261	C8 Octahydrobenzothiophene	2.03E-08
262	C9 Thiophene	1.52E-06
263	C9 Tetrahydropyrrole	0
264	C12 Iso paraffin with multiple branch	1.69E-03
265	C8 Octahydroindole	0
266	C11 Benzene	1.40E-02
267	C12 Iso olefin with one branch	0
268	C10 Tetralin	9.06E-04
269	N5_1_C12	0
270	C11 Decalin	1.04E-02
271	C12 Iso paraffin with one branch	2.94E-02
272	C10 Indane	3.11E-04
273	C9 Octahydrobenzothiophene	4.37E-08
274	C9 Tetrahydrothiophene	1.31E-07
275	C12 Normal olefin	0
276	C9 Octahydroindole	6.52E-05
277	C10 Indene	0
278	C12 Normal paraffin	3.05E-02
279	C9 Pyrridine	0
280	C8 Dihydrobenzothiophene	4.24E-16
281	C10 Naphthalene	0
282	C13 Iso paraffin with one branch	1.94E-02
283	C11 Indane	5.65E-04
284	C8 Pyrrole	0
285	C12 Cyclohexane	0
286	C10 Thiophene	1.08E-06
287	C9 Sulfide/mercaptan	1.99E-09
288	C10 Tetrahydropyrrole	0
289	C12 Benzene	1.58E-02

290	C13 Iso paraffin with multiple branch	1.63E-03
291	C8 Benzothiophene	2.76E-06
292	C11 Tetralin	1.12E-03
293	C9 Tetrahydroquinoline	0
294	C13 Iso olefin with one branch	0
295	C13 Iso olefin with multiple branch	0
296	C12 Decalin	1.24E-02
297	C9 Dihydrobenzothiophene	3.32E-17
298	C10 Octahydroindole	0
299	C13 Normal olefin	0
300	C13 Normal paraffin	2.94E-02
301	C10 Pyrridine	0
302	C9 Quinolone	0
303	C10 Tetrahydrothiophene	1.40E-07
304	C11 Indene	0
305	C9 Pyrrole	0
306	C11 Tetrahydropyrrole	0
307	C14 Iso paraffin with multiple branch	1.55E-03
308	C13 Cyclohexane	2.98E-02
309	C12 Indane	1.07E-03
310	C10 Sulfide/mercaptan	6.36E-09
311	C9 Benzothiophene	4.48E-06
312	C11 Thiophene	1.15E-06
313	C14 Iso paraffin with one branch	9.97E-03
314	C12 Tetralin	2.05E-04
315	C11 Naphthalene	0
316	C10 Tetrahydroquinoline	0
317	C14 Iso olefin with multiple branch	0
318	C14 Iso olefin with one branch	0
319	C13 Decalin	1.88E-02
320	C11 Octahydroindole	0
321	C10 Octahydrobenzothiophene	4.68E-08
322	C10 Dihydrobenzothiophene	4.93E-16
323	C14 Normal olefin	0
324	C13 Benzene	5.42E-03
325	C8 Indole	0
326	C14 Normal paraffin	2.78E-02
327	C11 Pyrridine	0

328	C11 Tetrahydrothiophene	1.49E-07
329	C14 Bicyclohexyl	1.02E-02
330	C10 Pyrrole	0
331	C15 Iso paraffin with multiple branch	1.44E-03
332	C12 Tetrahydropyrrole	0
333	C12 Indene	0
334	C14 Cyclohexane	3.25E-02
335	C11 Sulfide/mercaptan	6.74E-09
336	C13 Indane	1.19E-03
337	C11 Tetrahydroquinoline	0
338	C10 Benzothiophene	3.21E-06
	Total	**1**

The other fractions in offshore crude oil (true boiling points＞260℃) are pseudo-components. Comparison results of heavy oil results are shown in Fig. S11.

260-270C*	0.0062
270-280C*	0.0277
280-290C*	0.0171
290-300C*	0.0250
300-310C*	0.0285
310-320C*	0.0219
320-330C*	0.0214
330-340C*	0.0340
340-350C*	0.0120
350-360C*	0.0295
360-370C*	0.0309
370-380C*	0.0293
380-390C*	0.0205
390-400C*	0.0196
400-410C*	0.0255
410-420C*	0.0182
420-430C*	0.0213
430-440C*	0.0198
440-450C*	0.0179
450-460C*	0.0205
460-480C*	0.0278
480-500C*	0.0279
500-520C*	0.0241
520-540C*	0.0217
540-560C*	0.0193
560-580C*	0.0128
580-600C*	0.0065
600-625C*	0.0063
625-650C*	0.0053
650-675C*	0.0000
675-700C*	0.0000
700-725C*	0.0000
725-750C*	0.0001
750-775C*	0.0000
775-800C*	0.0000
800-825C*	0.0000
825-850C*	0.0000
850+C*	0.0882

Fig. S11 The molecular composition reconstruction results of offshore crude oil heavy fractions

The total fractions of offshore Crude oil components are summarized in Table S8.

Table S8. The total fractions of offshore crude oil components

1	H2	0
2	H2S	0

3	NH3	0
4	Methane	0
5	C1 Light Paraffin	0
6	Ethene	0
7	C2 Light olefin	0
8	Ethane	0
9	C2 Light Paraffin	0
10	C3 Light olefin	0
11	Prop1ene	0
12	C3 Light Paraffin	0
13	Propane	0
14	2MePropane	0
15	2MeProp1ene	0
16	C4 Light olefin	0
17	But1ene	0
18	C4 Light Paraffin	0
19	Butane	0
20	tr2-Butene	0
21	cis2-Butene	0
22	22DiMePropane	0
23	C5 Iso paraffin with multiple branch	0
24	3MeBut1ene	0
25	C5 Iso paraffin with one branch	0
26	2MeButane	0
27	Pent1ene	0
28	2MeBut1ene	0
29	C5 Normal paraffin	0
30	Pentane	0.004665
31	C5 Normal olefin	0
32	C5 Iso olefin with one branch	0
33	Pent2ene	0
34	2MeBut2ene	0
35	33DiMeBut1ene	0
36	CPentane	0.000114
37	C5 Cyclohexane	0
38	22DiMeButane	0
39	3MePent1ene	0
40	4MePent1ene	0
41	23DiMeBut1ene	0
42	4MePent2ene	0

43	C6 Iso paraffin with multiple branch	0
44	23DiMeButane	0.000465
45	C6 Iso paraffin with one branch	0
46	2MePentane	5.95E-13
47	2MePent1ene	0
48	3MePentane	0.003879
49	Hex1ene	0
50	2EtBut1ene	0
51	C6 Iso olefin with multiple branch	0
52	C6 Normal olefin	0
53	Hex3ene	0
54	2MePent2ene	0
55	3MePent2ene	0
56	Hex2ene	0
57	Hexane	0.006055
58	C6 Normal paraffin	0
59	C6 Iso olefin with one branch	0
60	MeCPentane	0.000249
61	23DiMeBut2ene	0
62	C7 Iso paraffin with multiple branch	0.000272
63	22DiMePentane	0
64	Benzene	0.000123
65	C6 Benzene	0
66	24DiMePentane	1.12E-14
67	C6 Cyclohexane	0
68	CHexane	0
69	223TrMeButane	0
70	C7 Iso olefin with multiple branch	0
71	C4 Thiophene	9.43E-08
72	33DiMePentane	0
73	C4 Tetrahydropyrrole	0
74	11DiMeCPentane	8.63E-15
75	23DiMePentane	0.001965
76	C7 Iso olefin with one branch	0
77	C7 Iso paraffin with one branch	0.000272

78	2MeHexane	4.71E-14
79	3MeHexane	0.008972
80	13DiMeCPentane	0.001106
81	3EtPentane	0.000307
82	C7 Normal olefin	0
83	C4 Sulfide/mercaptan	1.15E-09
84	Heptane	0.007241
85	C7 Normal paraffin	0.000272
86	224TrMePentane	0
87	12DiMeCPentane	0.000207
88	H2O	0
89	MeCHexane	0
90	C7 Cyclohexane	0.001803
91	EtCPentane	5.62E-05
92	113TrMetCPentane	1.24E-14
93	C5 Tetrahydropyrrole	0
94	C8 Iso paraffin with multiple branch	0.000483
95	22DiMeHexane	0
96	C8 Iso olefin with multiple branch	0
97	124TrMetCPentane	1.11E-06
98	25DiMeHexane	1.19E-14
99	223TrMePentane	0
100	24DiMeHexane	0.001749
101	Toluene	0.000162
102	C7 Benzene	0
103	33DiMeHexane	0
104	C5 Thiophene	2.16E-07
105	234TrMePentane	0.00015
106	1Me3EtCPentane	0.000566
107	112TrMetCPentane	0.000989
108	233TrMePentane	0
109	C5 Pyrridine	0
110	23DiMeHexane	0.00082
111	2Me3EtPentane	0.000287
112	C8 Iso olefin with one branch	0
113	123TrMetCPentane	0.001684
114	2MeHeptane	0.003831
115	C8 Iso paraffin with one branch	0.000483
116	4MeHeptane	0.006738

117	34DiMeHexane	7.76E-05
118	3MeHeptane	0.000342
119	3Me3EtPentane	0
120	3EtHexane	0.002153
121	11DiMeCHexane	0
122	1Me1EtCPentane	0.000574
123	C4 Tetrahydrothiophene	6.24E-09
124	14DiMeCHexane	0
125	13DiMeCHexane	0
126	IsoPrCPentane	0.000192
127	C8 Normal olefin	0
128	1124TeMeCPentane	1.59E-06
129	225TrMeHexane	0
130	12DiMeCHexane	0
131	Octane	0.008156
132	C8 Normal paraffin	0.000483
133	1Me2EtPentane	0.000723
134	224TrMeHexane	0
135	C5 Sulfide/mercaptan	1.3E-09
136	11DiMe3EtCPentane	4.78E-05
137	13DiMe1EtCPentane	0.00026
138	1123TeMeCPentane	0.000705
139	C4 Pyrrole	0
140	C9 Iso olefin with multiple branch	0
141	244TrMeHexane	0
142	235TrMeHexane	3.59E-15
143	C6 Tetrahydropyrrole	0
144	PrCPentane	8.07E-05
145	C8 Cyclohexane	0.010371
146	EtCHexane	0
147	1125TeMeCPentane	0.001302
148	24DiMeHeptane	0.000231
149	22DiMeHeptane	0
150	223TrMeHexane	0
151	2Me4EtHeptane	0.001445
152	1Me1IsoPrCPentane	2.03E-14
153	25DiMeHeptane	0.00255
154	C6 Thiophene	6.08E-07
155	44DiMeHeptane	0
156	114TrMeCHexane	0
157	1122TeMeCPentane	0.001888
158	26DiMeHeptane	0.001181

159	35DiMeHeptane	0.000818
160	EtBenzene	4.08E-15
161	C8 Benzene	0
162	C9 Iso paraffin with multiple branch	0.000969
163	24DiMe1EtCPentane	0.002318
164	N5_1_C9	0
165	113TrMeCHexane	0
166	33DiMeHeptane	0
167	11DiMe2EtCPentane	0.002517
168	12DiMe1EtCPentane	0.002491
169	233TrMeHexane	0
170	2Me3EtHeptane	0.000487
171	PXylene	0.000298
172	C5 Tetrahydrothiophene	1.42E-08
173	234TrMeHexane	2.34E-05
174	MXylene	0.000523
175	334TrMeHexane	0
176	1Me13IsoPrCPentane	0.000801
177	13DiMe2EtCPentane	0.001983
178	12DiMe3EtCPentane	0.002289
179	13DiEtCPentane	0.000987
180	1Me3PrCPentane	0.001293
181	4Me3EtHeptane	0.000286
182	3Me3EtHeptane	0
183	34DiMeHeptane	0.000159
184	135TrMeCHexane	0
185	23DiMeHeptane	7.74E-05
186	C9 Iso olefin with one branch	0
187	4EtHeptane	5.35E-14
188	124TrMeCHexane	0
189	1Me2IsoPrCPentane	0.002863
190	3EtHeptane	0.006507
191	2MeOctane	0.006861
192	C9 Iso paraffin with one branch	0.000508
193	3MeOctane	0.004968
194	C6 Pyrridine	0
195	OXylene	0.000167
196	4MeOctane	0.00134
197	1IsoButCPentane	0.001859
198	112TrMeCHexane	0

199	C9 Normal olefin	2.66E-05
200	1Me2PrCPentane	0.000732
201	12DiEtCPentane	0.000528
202	C6 Tetrahydrothiophene	1.59E-08
203	C5 Pyrrole	0
204	3Me1EtCHexane	0
205	1Me1PrCPentane	0.000257
206	11DiEtCPentane	0.000174
207	2SecBuCPentane	0.0006
208	4Me1EtCHexane	0
209	1SecBuCPentane	0.000132
210	Nonane	0.008774
211	C9 Normal paraffin	0.000508
212	123TrMeCHexane	0
213	2Me1EtCHexane	0
214	1Me1EtCHexane	0
215	IsoPrBenzene	0.000247
216	C6 Sulfide/mercaptan	1.94E-09
217	IsoPrCHexane	0
218	C7 Tetrahydropyrrole	0
219	C10 Iso olefin with multiple branch	0
220	BuCPentane	0.000116
221	PrCHexane	0
222	C9 Cyclohexane	0
223	C10 Iso paraffin with multiple branch	0.006901
224	C7 Thiophene	4.03E-07
225	PrBenzene	0.00033
226	C9 Benzene	0
227	4Me1EtBenzene	0.000615
228	3Me1EtBenzene	0.000607
229	N5_1_C10	0
230	135TrmeBenzene	0.000379
231	2Me1EtBenzene	0.000185
232	C10 Iso olefin with one branch	0
233	C10 Iso paraffin with one branch	0.01773
234	C7 Pyrridine	0
235	124TrmeBenzene	8.15E-05
236	C10 Normal olefin	0
237	C10 Cyclohexane	0

238	C7 Tetrahydrothiophene	2.63E-08
239	C8 Thiophene	4.39E-07
240	C10 Normal paraffin	0.009335
241	123TrmeBenzene	2.95E-05
242	C11 Iso paraffin with multiple branch	0.002168
243	C7 Sulfide/mercaptan	1.6E-09
244	C9 Indane	6.45E-05
245	C8 Tetrahydropyrrole	0
246	N5_1_C11	0
247	C10 Benzene	0.006712
248	C11 Iso olefin with one branch	0
249	C11 Iso olefin with multiple branch	0
250	C10 Decalin	0.002614
251	C11 Iso paraffin with one branch	0.015121
252	C8 Pyrridine	0
253	C9 Indene	0
254	C12 Iso olefin with multiple branch	0
255	C11 Normal olefin	0
256	C8 Tetrahydrothiophene	3.81E-08
257	C11 Normal paraffin	0.009601
258	C11 Cyclohexane	0
259	C7 Pyrrole	0
260	C8 Sulfide/mercaptan	1.73E-09
261	C8 Octahydrobenzothiophene	6.35E-09
262	C9 Thiophene	4.74E-07
263	C9 Tetrahydropyrrole	0
264	C12 Iso paraffin with multiple branch	0.00053
265	C8 Octahydroindole	0
266	C11 Benzene	0.004374
267	C12 Iso olefin with one branch	0
268	C10 Tetralin	0.000284
269	N5_1_C12	0
270	C11 Decalin	0.003271
271	C12 Iso paraffin with one branch	0.009199

272	C10 Indane	9.72E-05
273	C9 Octahydrobenzothiophene	1.37E-08
274	C9 Tetrahydrothiophene	4.1E-08
275	C12 Normal olefin	0
276	C9 Octahydroindole	2.04E-05
277	C10 Indene	0
278	C12 Normal paraffin	0.00955
279	C9 Pyrridine	0
280	C8 Dihydrobenzothiophene	1.33E-16
281	C10 Naphthalene	0
282	C13 Iso paraffin with one branch	0.006079
283	C11 Indane	0.000177
284	C8 Pyrrole	0
285	C12 Cyclohexane	0
286	C10 Thiophene	3.39E-07
287	C9 Sulfide/mercaptan	6.22E-10
288	C10 Tetrahydropyrrole	0
289	C12 Benzene	0.004948
290	C13 Iso paraffin with multiple branch	0.000511
291	C8 Benzothiophene	8.65E-07
292	C11 Tetralin	0.000351
293	C9 Tetrahydroquinoline	0
294	C13 Iso olefin with one branch	0
295	C13 Iso olefin with multiple branch	0
296	C12 Decalin	0.003881
297	C9 Dihydrobenzothiophene	1.04E-17
298	C10 Octahydroindole	0
299	C13 Normal olefin	0
300	C13 Normal paraffin	0.009201
301	C10 Pyrridine	0
302	C9 Quinolone	0
303	C10 Tetrahydrothiophene	4.38E-08
304	C11 Indene	0
305	C9 Pyrrole	0
306	C11 Tetrahydropyrrole	0
307	C14 Iso paraffin with multiple branch	0.000484
308	C13 Cyclohexane	0.009329

309	C12 Indane	0.000334
310	C10 Sulfide/mercaptan	1.99E-09
311	C9 Benzothiophene	1.4E-06
312	C11 Thiophene	3.6E-07
313	C14 Iso paraffin with one branch	0.00312
314	C12 Tetralin	6.43E-05
315	C11 Naphthalene	0
316	C10 Tetrahydroquinoline	0
317	C14 Iso olefin with multiple branch	0
318	C14 Iso olefin with one branch	0
319	C13 Decalin	0.005871
320	C11 Octahydroindole	0
321	C10 Octahydrobenzothiophene	1.46E-08
322	C10 Dihydrobenzothiophene	1.54E-16
323	C14 Normal olefin	0
324	C13 Benzene	0.001696
325	C8 Indole	0
326	C14 Normal paraffin	0.008713
327	C11 Pyrridine	0
328	C11 Tetrahydrothiophene	4.65E-08
329	C14 Bicyclohexyl	0.003206
330	C10 Pyrrole	0
331	C15 Iso paraffin with multiple branch	0.000451
332	C12 Tetrahydropyrrole	0
333	C12 Indene	0
334	C14 Cyclohexane	0.010182
335	C11 Sulfide/mercaptan	2.11E-09
336	C13 Indane	0.000373
337	C11 Tetrahydroquinoline	0
338	C10 Benzothiophene	1.01E-06
339	**260-270C***	**6.22E-03**
340	**270-280C***	**2.77E-02**
341	**280-290C***	**1.71E-02**
342	**290-300C***	**2.50E-02**
343	**300-310C***	**2.85E-02**
344	**310-320C***	**2.19E-02**
345	**320-330C***	**2.14E-02**
346	**330-340C***	**3.40E-02**

347	**340-350C***	**1.20E-02**
348	**350-360C***	**2.95E-02**
349	**360-370C***	**3.09E-02**
350	**370-380C***	**2.93E-02**
351	**380-390C***	**2.05E-02**
352	**390-400C***	**1.96E-02**
353	**400-410C***	**2.55E-02**
354	**410-420C***	**1.82E-02**
355	**420-430C***	**2.13E-02**
356	**430-440C***	**1.98E-02**
357	**440-450C***	**1.79E-02**
358	**450-460C***	**2.05E-02**
359	**460-480C***	**2.78E-02**
360	**480-500C***	**2.79E-02**
361	**500-520C***	**2.41E-02**
362	**520-540C***	**2.17E-02**
363	**540-560C***	**1.93E-02**
364	**560-580C***	**1.28E-02**
365	**580-600C***	**6.54E-03**
366	**600-625C***	**6.27E-03**
367	**625-650C***	**5.32E-03**
368	**650-675C***	**3.24E-05**
369	**675-700C***	**2.29E-05**
370	**700-725C***	**1.32E-05**
371	**725-750C***	**5.13E-05**
372	**750-775C***	**4.87E-05**
373	**775-800C***	**1.22E-05**
374	**800-825C***	**6.02E-08**
375	**825-850C***	**0**
376	**850+C***	**8.82E-02**
	Total	**1.00**

We compared and verified the distillation curve and density of the total fraction of offshore crude before and after molecular modification. These results are shown in Table S9. It can be seen from Table S8 that the relative error between the distillation curve and the density of the total fraction of crude oil before and after molecular reconstruction is less than 5.0%. The accuracy of offshore crude oil's complete fraction property reconstruction can be further verified.

Table S9. Comparison results of total fractions of offshore crude oil before and after reconstruction

Items	Total fractions of offshore crude oil before molecular reconstruction	Total fractions of offshore crude oil after molecular reconstruction	relative errors %
Initial boiling point/℃	62.25947	65.45	5.124562
10%/℃	133.7269	135.565	1.374541
30%/℃	230.7564	245.6876	6.470568
50%/℃	326.2554	342.453	4.964692
70%/℃	405.5753	417.567	2.956722
90%/℃	532.2289	543.65	2.145904
Final boiling point/℃	905.5129	891.435	1.55468
Density (kg/m_3)	781.45	786.25	0.624435

1.2. Process simulation

1.2.1 Reaction network description

Actually, the FCC in Aspen HYSYS is a state-of-the-art Fluidized Catalytic Cracking Unit simulation system that can be used for modeling an FCC unit as a standalone unit operation or as part of a refinery-wide flowsheet. It includes a feed characterization system, regenerator(s), a reactor, riser(s), and a product delumper. The riser, reactor, and regenerator are rigorous, kinetic-based models. The feed characterization system and product delumper are designed to work together with the HYSYS assay system so the FCC model can be simulated in a refinery-wide flowsheet. The FCC Reactor model also includes a number of models to account for coke formation and its transmittal through the mass flow paths. Models for handling the distribution of feed sulfur and nitrogen among the gas plant products are also provided. The Aspen HYSYS FCC model kinetics are derived from the Mobil ten-lump mechanism. The FCC Reactor has expanded the number of reactant/product lumps to 21 and changed the functionality of several key lumps. The reactions themselves are all based on well-understood first-order kinetics that all occur in the vapor phase. The kinetic expressions are integrated along the length of the riser and are dependent on the catalyst bulk density, coke on the catalyst, MAT activity, essential nitrogen, and metals content. The MAT activity and basic nitrogen are entered from external model sources and affect the riser kinetics uniformly. The catalyst bulk density and coke on the catalyst are also integrated along the riser length and are themselves a function of pressure drop, coke makes, and molar expansion. The pressure drop includes elements of head, friction, and acceleration.

All kinetics in the reactor are based on the 21-lump kinetic system. The reaction pathways represent paraffinic cracking, naphthenic ring-opening, alkyl side chain cracking, ring condensation, kinetic coke made from typical condensation reactions, and metals coke make due to dehydrogenation. The reaction paths have been logically grouped to make yield parameterization more convenient. Thus all the pathways which lead to gas make up one class, the gasoline pathways make up another class, and so on.

In this way, with only a small number of yield measurements of the operation unit, the kinetic rate parameters for the more than fifty reaction pathways can be easily tuned to match the unit yields. To match the specific product compositions that are observed on the unit (provided that information is available), additional tuning of paraffinic and aromatic reaction rates must be performed. The detailed reaction networks are shown in Fig. S12 and Fig. S13 [3, 4].

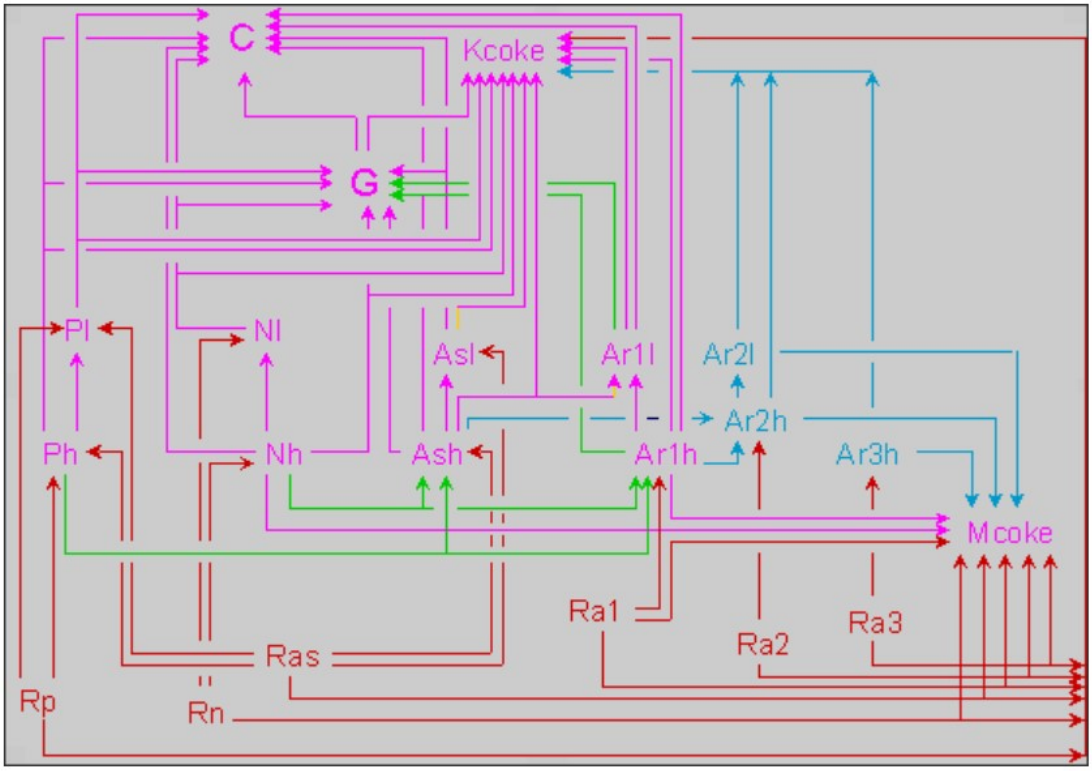

Fig. S12 Schematic for the 21-Lump Reaction Paths

No.	Lump	NBP Range	Description
1	C		C lump – produces light gases
2	G	< 430 °F	Gasoline Lump C5
3	Pl	430 – 650 °F	Light Paraffins
4	Nl		Light Naphthenes
5	Ar1l		Light 1-Ring Aromatics
6	Ar2l		Light 2-Ring Aromatics
7	Asl		Light Aromatic Ring Substituent Carbons
8	Ph	650 – 950 °F	Heavy Paraffins
9	Nh		Heavy Naphthenes
10	Ar1h		Heavy 1-Ring Aromatics
11	Ar2h		Heavy 2-Ring Aromatics
12	Ar3h		Heavy 3-Ring Aromatics
13	Ash		Heavy Aromatic Ring Substituent Carbons
14	Rp	> 950 °F	Resid Paraffins
15	Rn		Resid Naphthenes
16	Ra1		Resid 1-Ring Aromatics
17	Ra2		Resid 2-Ring Aromatics
18	Ra3		Resid 3-Ring Aromatics
19	Ras		Resid Aromatic Ring Substituent Carbons
20	Kcoke	N/A	Kinetic Coke
21	Mcoke		Metals Coke

Fig. S12 Schematic for the 21-Lump Reaction Paths (continued)

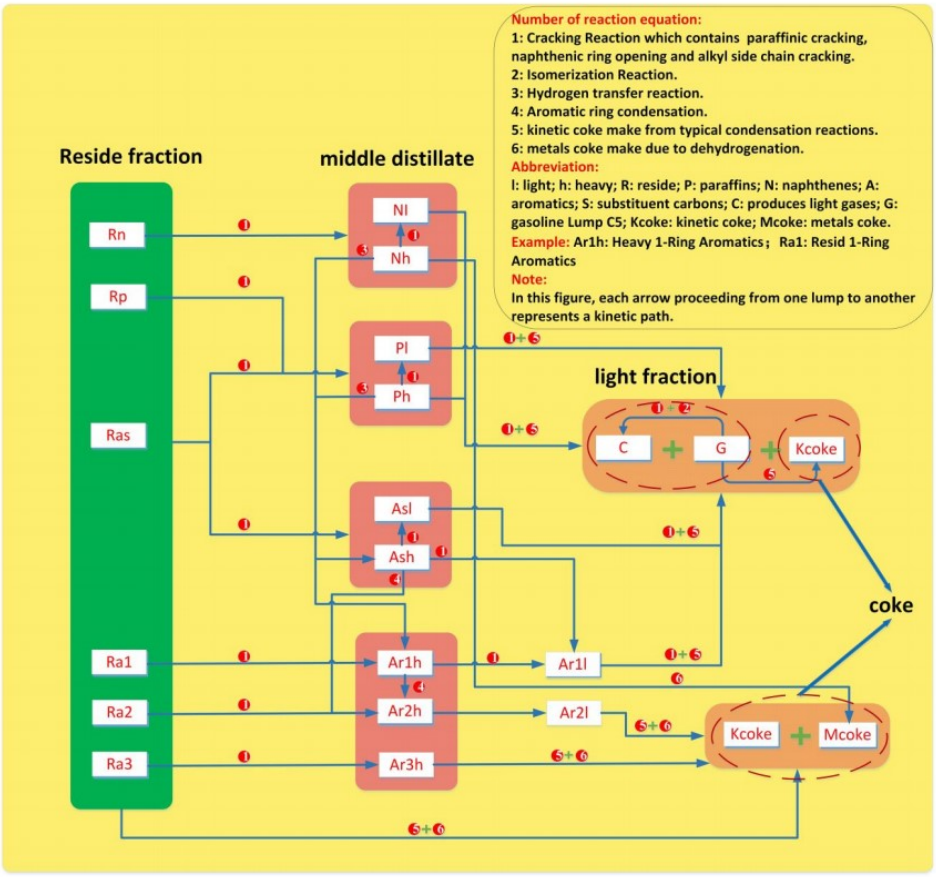

Fig. S13. The 21-lump kinetic model and network of kinetic reaction pathways.

This system divides the reactants and products into lumped aggregates of material classified by chemical type and boiling point range. These lumps are similar to pseudo-components but are based on the molecular structure in addition to the boiling range for typical pseudo-component breakdowns. The molecular structures selected are based on likely reaction pathways, and mechanisms understood to exist in fluid catalytic cracking chemistry. The table below summarizes the lumps used in the model. These lumps are classified into paraffinic, naphthenic, and aromatic chemicals, as shown in Fig. S10. Aromatics are further divided into substituent carbons and ring aromatic carbons. The components were also selected to represent convenient boiling ranges representing yields of light gases, gasoline, light cycle oil, heavy cycle oil, and the main fractionator bottoms (including any remaining resid). The light gas components represent all light gases from H_2 to C_5. The gasoline component represents the component range from C_5 to 430 °F.

After the amounts of these chemicals are determined from the correlation, the riser

effluent is split up into even finer compositional detail. This split of the C4=, C5=, iC5, and the C6 to 430 °F gasoline are split into the isomers. The amount of each isomer created is determined by fixed ratios or calibration factors. The ratios are tuned to match a particular unit by adjusting calibration factors for each isomer. The amount of each isomer created is determined by fixed ratios or calibration factors. The ratios are tuned to match a particular unit by adjusting calibration factors. The calibration factors are determined in a calibration run. The calibration run is the most important step in developing FCC models. Many scholars have applied calibration run and developed Aspen HYSYS FCC models to simulate the actual models of catalytic cracking in refineries [3, 5, 6]. We have also developed some novel crude oil or heavy oil catalytic cracking processes to further verify the accuracy of the proposed FCC models [4, 7-12].

1.2.2 Process modeling and verification

In this study, the proposed processes' processing capacity is 3.0 Mt/year. Metal oxide catalysts are employed in the OCOCC process. The direct catalytic cracking of sulfur crude oil is carried out in a pilot-scale catalytic cracking unit, which consists of the riser reactor, catalyst stripper, regenerator and product separation system, as illustrated in Fig. S14. The pilot-scale catalytic cracking unit could carry out continuous cracking reaction and catalyst regeneration operation similar to the commercial catalytic cracking unit. The computer controls the display and adjustment of main operation parameters.

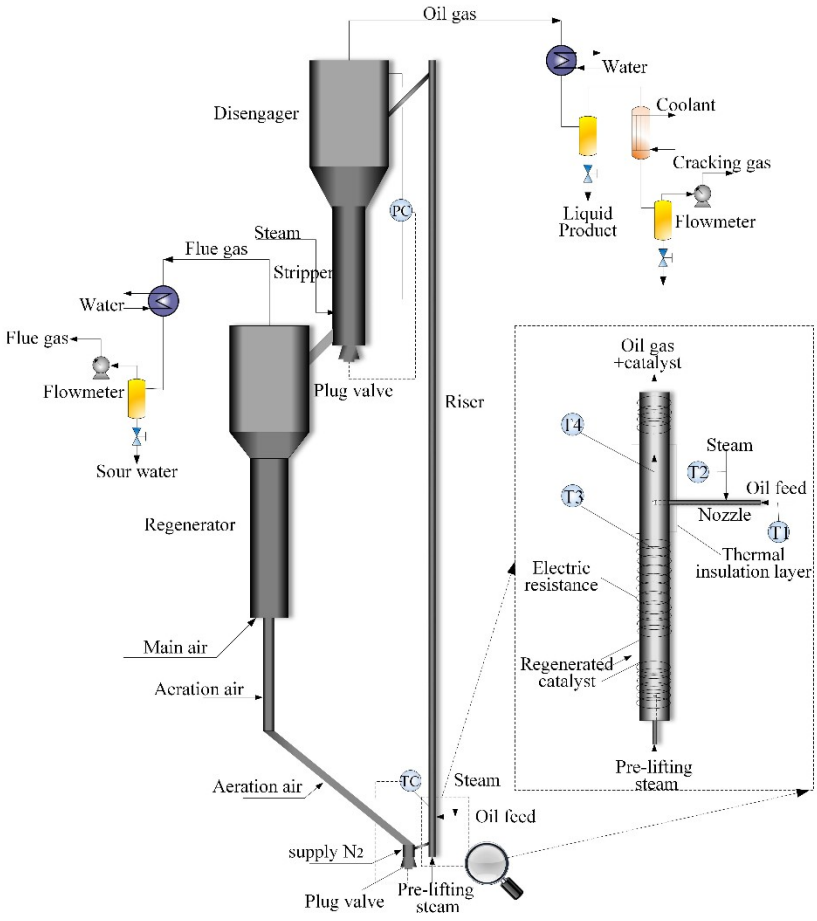

Fig. S14. Schematic flowsheet of the pilot-scale crude oil catalytic cracking unit.

The geometric dimension parameters of the two-stage catalytic cracking reactor in the OCOCC processes are listed in Table S10.

Table S10. The geometric dimension parameters in the OCOCC proceess

Item	Geometry
Riser 1#	
Total length/m	28.00
Diameter/m	0.69
Riser 2#	
Total length/m	28.00
Diameter/m	0.56
Riser termination zone	
Length/m	1.20
Diameter/m	6.70
Catalyst Stripper	
Height/m	6.00
Diameter/m	3.35
Annulus Diameter/m	3.35
Regenerator	
Dense Bed Height/m	4.00
Dense Bed Diameter/m	8.20
Dilute Phase Diameter/m	8.20
Interface Diameter/m	8.20
Cyclone Inlet Height/m	12.70
Cyclone Inlet Diameter/m	1.50
Cyclone Outlet Diameter/m	1.50

The calibration factors adopted in this work is shown in Table S11.

Table S11. The calibration parameters in the OCOCC processes.

Item	OCOCC process
Activity on Pathways to C Lump	2.42800000000000
Activity on Pathways to G Lump	-3.47980693824210
Activity on Pathways to L Lump	1.11026989435714
Metals Coke Activity	1.02005146783840e-002
Catalyst Deactivation Factor	0.510871737076991
Catalyst Surface Area Parameter	-10.1351351351351
Effluent per Mass of Catalyst into Stripper	115.986035481736
Stripper Parameter	-0.246530721670274
H to C Ratio for Coke	1.01104701375606
Coke Burn Activity	32.9352229325014
CO Heterogeneous Burn Activity	-0.566446898418394
CO Homogeneous Burn Activity	9.41117504750300
Heat of Cracking Parameter	0.265564432657067
Kinetic Coke Activity Factor	-7.66461384315751e-002

The detailed simulation process flowsheet of the OCOCC process in Aspen HYSYS is illustrated in Fig. S15-S16. Detailed process operating parameters of key columns in the OCOCC processes are listed in Table S12.

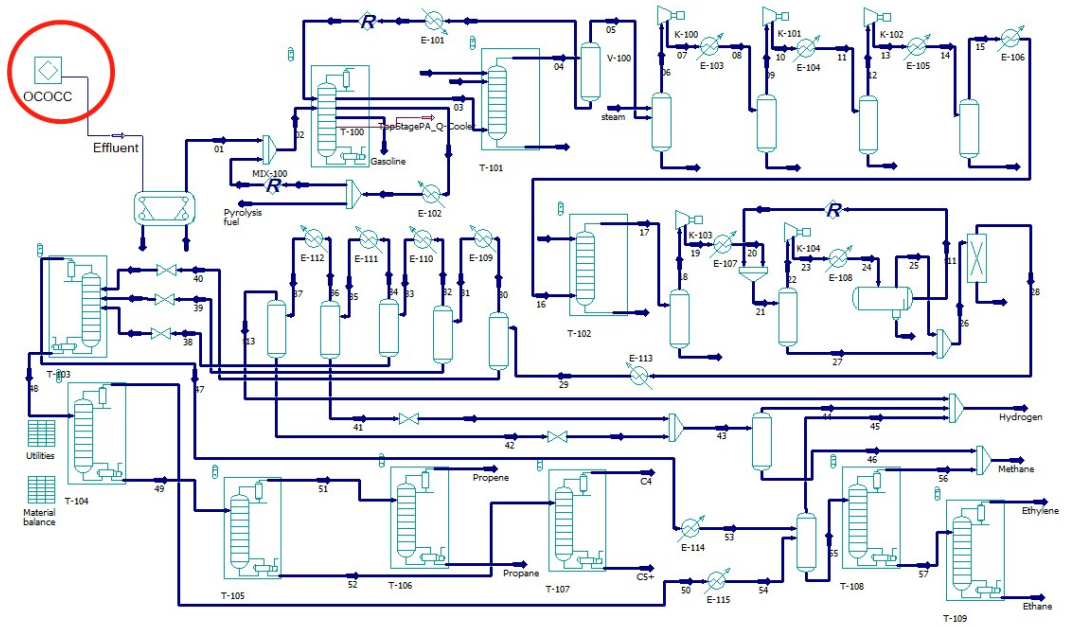

Fig. S15. The detailed simulation process separation flowsheet of OCOCC process in Aspen HYSYS.

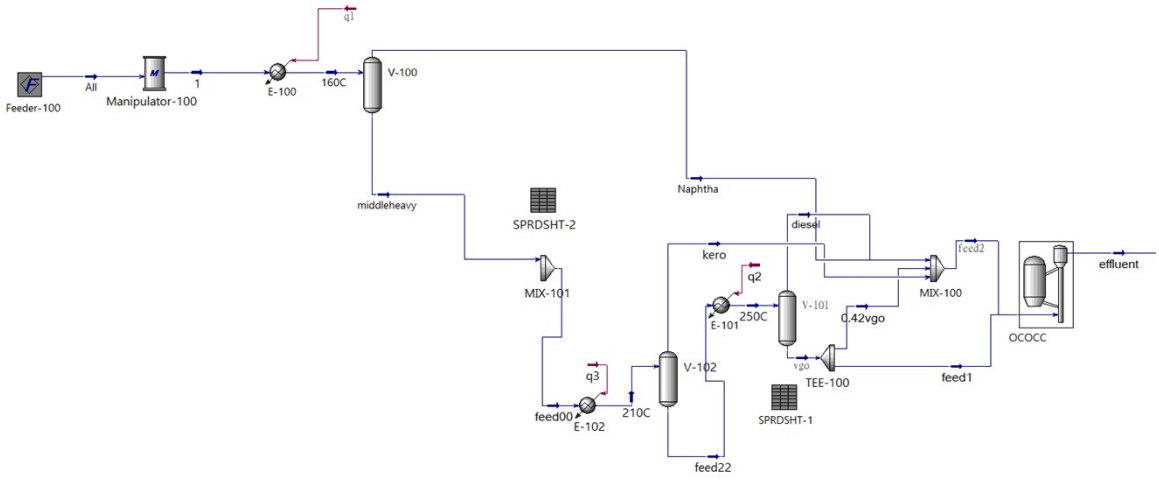

Fig. S16. The detailed simulation process reaction flowsheet of OCOCC process in Aspen HYSYS (The sub-process of OCOCC-React in Fig S15.)

The operating parameters of critical columns in the OCOCC processes are listed in Table S12.

Table S12. Operating parameters of critical columns in the OCOCC processes.

Columns	The OCOCC process	
	Temperature (℃)	Pressure (MPa)
T-100	[124.3, 338.2]	[0.142, 0.156]
T-101	[68.2, 107.1]	[0.132, 0.146]
T-102	[42.2, 43.2]	[0.932, 1.046]
T-103	[-73.1, -9.3]	[0.562, 0.577]
T-104	[15.7, 109.3]	[3.562, 3.693]
T-105	[78.3, 146.3]	[3.458, 3.572]
T-106	[73.1, 87.3]	[3.172, 3.466]
T-107	[134.3, 217.5]	[3.023, 3.263]
T-108	[-98.2, -9.2]	[3.133, 3.173]
T-109	[-34.3, -10.4]	[1.762, 3.242]

1.3. The source code used to execute the many-objective optimization strategy

The compressed source code document connected between HYSYS and Python 3.8 is shown in Fig. 17. The original code list is also given. The detailed steps of performing the NSGA-III are also available in this supporting information.

```
7
8   from win32com.client import Dispatch
9
10  # Create the HYSYS COM object and open HYSYS V12.0.
11  HYSYSApp = Dispatch("HYSYS.Application.V12.0")
12  HYSYSApp.Visible = True
13
14  # Open the simulation case.
15  HYSYSCase = HYSYSApp.SimulationCases.Open("C:\HYSYS.hsc")
16  HYSYSCase.Visible = True
17
18  HYSYSCase.Solver.CanSolve = False
19
20  # Navigate to the Main flowsheet.
21  mainFlowsheet = HYSYSCase.Flowsheet
22
23
24
25  HYSYSCase.Solver.CanSolve = False
26  Spreadsheet = mainFlowsheet.Operations.Item("Spreadsheet")
27
28  # Set the CellValue
29  hyCell = Spreadsheet.Cell(0, 0)
30  hyCell.CellValue = 111
31  value = hyCell.CellValue
32  unit = hyCell.Units
33  print("The value of cell A1 is", value, unit)
34
35  # Get the CellValue
36  hyCell = Spreadsheet.Cell(1, 1)
37  value = hyCell.CellValue*3600
38  unit = hyCell.Units
39  print("The value of cell A2 is", value, unit)
40
41  # HYSYSCase.Solver.CanSolve = True
42  # # Get the FORMULA
43  # hyCell = Spreadsheet.Cell(0, 2)
44  # FORMULA = hyCell.CellText
45  # value = hyCell.CellValue
46  # unit = hyCell.Units
47  # print("The FORMULA is", FORMULA, "and the value is", value, unit)
```

Fig. S17. The code of combining Aspen HYSYS-Python Interface

```
# -*- coding: utf-8 -*-
"""
Created on Sun Dec  5 16:52:07 2022
```

```
@author: zhouxin
"""
from win32com.client import Dispatch

# Create the HYSYS COM object and open HYSYS V12.0.
HYSYSApp = Dispatch("HYSYS.Application.V12.0")
HYSYSApp.Visible = True
# Open the simulation case.
HYSYSCase = HYSYSApp.SimulationCases.Open("C:\HYSYS.hsc")
HYSYSCase.Visible = True
HYSYSCase.Solver.CanSolve = False

# Navigate to the Main flowsheet.
mainFlowsheet = HYSYSCase.Flowsheet



HYSYSCase.Solver.CanSolve = False
Spreadsheet = mainFlowsheet.Operations.Item("Spreadsheet")

# Set the CellValue
hyCell = Spreadsheet.Cell(0, 0)
hyCell.CellValue = 111
value = hyCell.CellValue
unit = hyCell.Units
print("The value of cell A1 is", value, unit)
# Get the CellValue
hyCell = Spreadsheet.Cell(1, 1)
value = hyCell.CellValue*3600
unit = hyCell.Units
print("The value of cell A2 is", value, unit)
# HYSYSCase.Solver.CanSolve = True
# # Get the FORMULA
# hyCell = Spreadsheet.Cell(0, 2)
# FORMULA = hyCell.CellText
# value = hyCell.CellValue
# unit = hyCell.Units
# print("The FORMULA is", FORMULA, "and the value is", value, unit)
```

How to perform the NSGA-III

Pip Instal

```
pip install -U pymoo
```

```
from pymoo.algorithms.moo.nsga3 import NSGA3
```

Ultimately, the Pareto optimal solution set is achieved through the process of optimization calculation by considering the relationship and range of variation between the objective and constraint functions. The programming implementation process of NSGA-III adopted in this research has been shared on the personal homepage of the GitHub website. The specific execution steps (pseudo code) of the algorithm are shown in Figure 11a. The program steps of the joint Aspen HYSYS and NSGA-III intelligent optimization algorithm implemented in this research are shown in Figure 11b (the code is compiled by Python v3.8). All process simulations and multi-objective optimization of the OCOCC process in this work are carried out on the ThinkPad X1-Carbon laptop. The environment and conditions for multi-objective optimization are as follows: (1) Operating system: Windows 11 64 bit; (2) CPU: Intel (R) Core (TM) i7-1165 G7; (3) Running memory: 16GB. See the Supporting Materials for the communication link code between Aspen HYSYS simulation software and Spyder compiler.

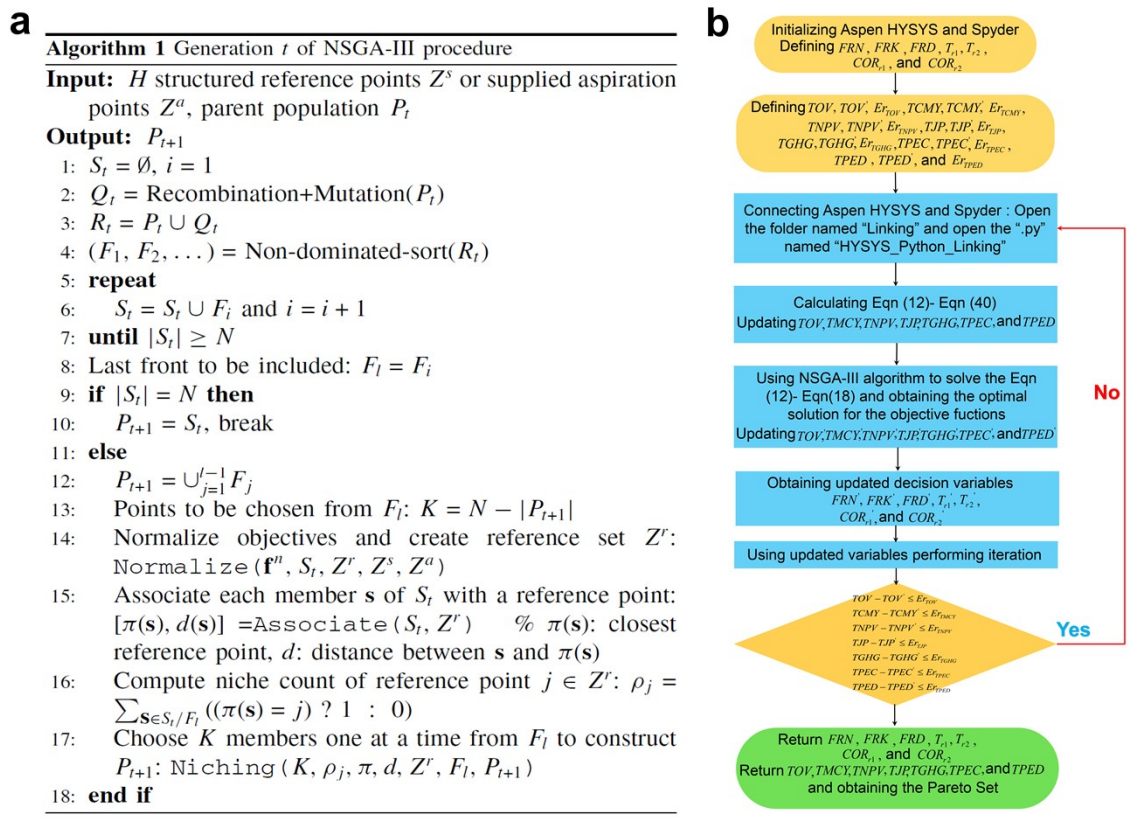

Figure S18. (a) NSGA-III intelligent optimization algorithm execution diagram; (b) Aspen HYSYS and Python jointly implement NSGA-III intelligent optimization algorithm to achieve multi-objective optimization

The Pareto set

No.	FT/℃	HC/wt%	FNR	FKR	FDR	T_{r1}	T_{r12}	COR_{r1}	COR_{r12}
1	178.37	1.56	189.97	216.31	230.56	629.57	677.38	12.26	16.46
2	178.20	1.52	150.89	210.66	233.72	621.85	674.01	11.85	16.76
3	150.93	1.44	150.01	199.30	234.24	621.91	676.26	12.65	17.78
4	151.75	1.44	189.48	201.20	245.93	631.64	671.66	10.25	16.04
5	168.50	1.59	188.01	206.70	257.47	632.83	667.80	12.43	18.02
6	165.52	1.57	181.61	208.46	246.32	633.08	662.93	10.30	16.11
7	161.19	1.58	185.04	198.60	257.30	621.91	663.72	13.87	16.90
8	178.20	1.52	185.15	210.66	256.90	621.91	674.01	13.99	16.76
9	151.84	1.45	187.20	200.39	241.09	639.22	676.73	13.31	17.74
10	170.61	1.58	179.99	215.10	246.57	633.08	661.24	10.30	16.11
11	152.15	1.52	183.54	216.37	241.49	629.57	670.67	13.44	16.43
12	172.77	1.44	150.01	212.21	240.50	637.83	675.32	12.65	17.81
13	165.54	1.54	150.01	199.31	236.86	621.85	675.77	14.02	15.87
14	161.17	1.52	150.05	199.00	241.08	638.97	675.90	11.71	16.79
15	170.53	1.58	156.89	194.03	257.98	633.94	661.32	10.38	19.12

16	151.86	1.43	181.18	213.76	257.53	639.16	677.13	13.50	18.16
17	174.70	1.55	154.14	210.61	242.38	621.85	679.28	12.33	16.20
18	168.76	1.46	150.21	196.52	256.81	627.92	674.10	12.15	16.65
19	156.34	1.52	189.28	215.13	238.36	630.69	671.30	12.64	16.47
20	178.27	1.57	181.61	208.33	233.93	633.08	662.93	10.31	16.09
21	152.14	1.47	179.88	199.43	238.95	639.38	663.50	11.70	18.82
22	177.13	1.47	181.90	199.37	245.94	639.94	677.09	11.70	16.11
23	177.05	1.54	187.74	199.32	236.83	621.32	675.73	14.02	16.92
24	165.52	1.57	179.36	198.90	246.32	633.08	662.93	10.30	16.11
25	165.69	1.55	187.20	216.31	241.49	629.57	675.19	13.31	16.46
26	154.07	1.52	150.98	207.49	234.13	637.86	663.14	12.65	19.04
27	166.06	1.55	187.15	197.72	231.39	623.39	662.66	14.27	17.72
28	151.75	1.44	189.04	201.70	244.88	631.17	679.36	10.24	16.17
29	152.61	1.43	150.01	212.21	240.51	629.12	670.38	12.66	16.54
30	178.68	1.58	153.25	211.22	257.98	634.91	678.18	10.36	19.25
31	157.77	1.52	150.01	206.62	257.73	621.85	673.89	12.03	19.04
32	150.93	1.44	152.82	208.86	234.24	621.91	676.26	12.65	17.49
33	155.80	1.52	150.25	207.49	245.47	622.29	663.14	12.61	16.34
34	177.05	1.54	150.22	199.34	232.33	620.65	675.73	13.41	16.92
35	155.80	1.52	150.25	207.49	238.49	622.05	663.14	12.65	19.04
36	161.20	1.43	152.45	196.19	250.69	633.19	666.80	10.02	16.13
37	176.96	1.52	152.52	201.46	242.29	633.08	676.64	11.82	16.10
38	152.25	1.50	152.73	201.46	242.29	632.81	663.05	11.82	16.10
39	178.76	1.58	179.99	215.10	246.57	633.08	679.04	10.30	16.11
40	159.94	1.52	150.50	199.00	241.08	638.97	676.50	11.71	16.79

Assessment of the solution set

The Hypervolume indicator calculates the volume of the region dominated by a set of solutions in the objective space. It considers both the number and quality of non-dominated solutions in the set. A larger Hypervolume value indicates that the solution set covers a larger, better area in the objective space. The hypervolume indicator provides a comprehensive assessment of a set of solutions by measuring the volume of the objective space dominated by these solutions. This means it takes into account both the convergence to the Pareto-optimal front and the diversity of the solutions. [15] The

calculated HV value is 0.9215874. The value being close to 1 indicates that the obtained set of solutions demonstrates good overall performance in terms of convergence and diversity.

2. Techno-economic analysis and estimation parameters

From a detailed techno-economic point of view, net present value (NPV), and internal rate of return (IRR), the OCOCC processes are compared comprehensively. Raw materials, utilities, employee welfare and maintenance management expenses are included in the total operating expenses. Utility costs, including power, steam, cooling water, gas, refrigerant, etc., are calculated according to the energy balance simulated by Aspen HYSYS. This study considers two financial evaluation indexes: NPV and IRR. NPV and IRR can be calculated by Eqn S1-Eqn S3, respectively [7-10].

$$NCF_y = TPR_y - FC_y - VC_y \tag{S1}$$

$$NPV = \sum_{y=0}^{WPL} \frac{NCF_y}{(1+d_r)^y} \tag{S2}$$

$$0 = \sum_{y=0}^{WPL} \frac{NCF_y}{(1+IRR)^y} \tag{S3}$$

where NCF means the net cash flow in the year y; TPR_y represents the total project revenue; TFC_y and TVC_y represent the total fixed cost and total variable cost in the year y; d_r is the discount rate, 10%; and PL means the plant life, 20 years.

Table S13. Feedstock and product prices [13]

Items	Price (USD/ton)
Offshore crude oil	**639.5**
Methane/Dry gas	416.5
Ethylene	1183.1
Propylene	1166.2
Propane	777.1
Ethane	686.7
C_4	960.8
gasoline (RON: 113)	1547.4
diesel	768.5
heavy oil	691.5

Based on Brent crude oil price 80 $/bbl.

Table S14. Cost parameters and assumptions for process economic evaluation. [13,14]

Items	Base value	Items	Base value
Make up water	0.42 USD/t	Operating time	8400h
Recycling cooling water	0.05 USD/t	Production load	100%
Steam	21.44 USD/t, Low pressure 22.54 USD/t, Middle pressure 23.63 USD/t, High pressure	Project construction period	2 years
Power	0.12 USD/(kW·h)	Salaries	15000 USD/person/year
fuel oil/fuel gas	216.5 USD/t	Net salvage rate	3%
interest rate	8%	Project maintenance and management costs	3% of total direct capital cost
plant life span	20 years	discounted annual rate	15%
tax rate	25%	Benchmark IRR	≥12%

Based on Brent crude oil price 80 $/bbl.

Table S15. Summary of scale factors for estimating the capital cost.

Process	Capacities in base cases/(10kt/year)	Basic costs/(USD)	Scale factors	comprehensive adjustment factor	source
Crude oil catalytic cracking unit	150	4.20×10^{8}	0.8	1.02	[14]

3. Supplement to the research progress

Table 16. The state-of-the-art technology

Feedstocks	Process, reactors, and catalysts	Conditions	Yields of chemicals	$CH_4/C_{2=}$	Classification	Ref.
AL; AXL; ASL[a]	fixed-bed micro-activity test (MAT); Equilibrium FCC catalysts/ZSM-5	T: 600-650°C	**C_2-C_4 olefins yields: 39.1-42.9 wt%** Naphtha yields: 23.0-31.7wt%	0.26-0.64	COCC technology; Chemicals and fuels	*J ANAL APPL PYROL. 2020;145:104705*
ASL	riser simulator; USY and MFI zeolite	T: 500-575°C	**C_2-C_4 olefins yields: 10.0-26.8 wt%** Naphtha yields: 37.3-51.2wt%	0.14-0.43	COCC technology; Chemicals and fuels	*ENERG FUEL. 2018;32:2234-2244*
ASL	fixed-bed microactivity test; Equilibrium FCC catalysts/MFI	T: 550-650°C	**C_2-C_4 olefins yields: 11.6-34.9 wt%** Naphtha yields: 35.4-53.3wt%	0.11-0.63	COCC technology; Chemicals and fuels	*ENERG FUEL. 2018;32:6189-6199*
Light crude oil	Equilibrium FCC catalysts	T: 560-640°C	**C_2-C_4 olefins yields: 2.5-21.6 wt%** Naphtha yields: 40.2-44.8wt%	0.50-0.75	COCC technology; Chemicals and fuels	*FUEL. 2018;211:726-736*
AL; AXL; ASL	Microactivity test unit; Equilibrium FCC catalysts/MFI	T: 550°C	**C_2-C_4 olefins yields: 9.8-21.3 wt%** Naphtha yields: 29.8-59.9wt%	1.53-2.64	COCC technology; Chemicals and fuels	*Chemical Engineering Research and Design. 2017;120:121-137; ENERG FUEL. 2017;31:12677-12684*
AXL	fixed-bed microactivity test Equilibrium FCC catalysts/MFI	T: 550-650°C	**C_2-C_4 olefins yields: 22.8-32.7 wt%** Naphtha yields: 24.4-	0.38-0.69	COCC technology; Chemicals and	*ENERG FUEL. 2018;32:8705-8714*

			48.3wt%		fuels	
Crude oil[a]	Preheat+flash+catalytic cracking	T: 600-650°C; catalyst/oil: 20~31	**C_2-C_4 olefins yields: 23.0-31.3 wt%** Naphtha yields: 47.2-48.9wt%	0.60~0.63	COCC technology; Chemicals and fuels	*Saudi Arabian Oil Company*
Hydrotreated AL	Flash+conventional hydrotreating +slurry hydrtreating+steam cracking	T: 400-900°C; Steam/oil: 0.3~2	Ethylene: 23.2wt%; Propylene: 13.3wt% Butadiene: 4.9 wt%; Butene: 4.2 wt%	0.46~0.47	COSC technology; Chemicals	*Saudi Arabian Oil Company*
Alaskan crude oil	Thermal cracking tube	T: 829~843°C;	Ethylene: 19.3~20.4wt%; Propylene: 12.1~12.2wt%; Butadiene: 4.7 wt%;	0.46~0.47	COSC technology; Chemicals	*US Pat., 0016673A1*
AL	Thermal cracking tube	Steam/oil: 1.2	Ethylene: 18wt%; Propylene: 13.8wt%; Butadiene: 2.7 wt%; Butene: 2.9 wt%	0.56	COSC technology; Chemicals	*US Pat., 0097002A1*
Agbami crude oil	Thermal cracking tube	Steam/oil: 1.0	Ethylene:21.5wt%; Propylene: 12.9wt%; Butadiene: 4.0 wt%; Butene: 4.4 wt%	0.39	COSC technology; Chemicals	*US Pat., 0097002A1*

a: AL=Arab light; AXL=Arab extra light; ASL=Arab super light.

Table 17. A detailed review of two-stage riser catalytic cracking technology

Feedstocks	Process, reactors, and catalysts	Conditions	Yields of chemicals	$CH_4/C_{2=}$	Classification	Ref.
C4	pilot-scale riser FCC unit; HZSM-5+USY zeolite catalysts	T: 510°C; catalyst/oil: 8	Ethylene: 7.35wt%; Propylene: 28.7wt% Butene: 22.9 wt%; Gasoline: 14.8wt%	1.14	Two-stage FCC technology	*IND ENG CHEM RES. 2007;46:4914-4920*
Naphtha	pilot-scale riser FCC unit; Y zeolite equilibrium FCC catalysts	T: 480°C	**C_2-C_4 olefins yields: 11.88-17.22 wt%** Naphtha yields: 73.41-82.46wt%	N/A	Two-stage FCC technology	*IND ENG CHEM RES. 2013;52:6366-6376*
Diesel	pilot-scale riser FCC unit; HZSM-5+USY zeolite catalysts	T: 510-560°C; catalyst/oil: 5	**C_2-C_4 olefins yields: 2.64-19.30 wt%** Gasoline: 12.35-56.1wt%	N/A	Two-stage FCC technology	*ENERG FUEL. 2017;31:2749-2754;* ENERG FUEL. 2017;31:6968-6976
Vacuum gas oil	pilot-scale riser FCC unit; HZSM-5+USY zeolite catalysts	T: 500~550°C; catalyst/oil: 7~18	**C_2-C_4 olefins yields: 35.35-27.06 wt%** Naphtha yields: 22.11-43.29wt%	1.54-2.01	Two-stage FCC technology	*ENERG FUEL. 2013;27:654-665; ENERG FUEL. 2019;33:12106-12120*
Daqing residue	pilot-scale riser FCC unit; HZSM-5+USY zeolite catalysts	T: 510~580°C; catalyst/oil: 7~18	**C_2-C_4 olefins yields: 35.35-37.80 wt%** Naphtha yields: 25.04-26.86wt%	0.40-0.41	Two-stage FCC technology	*IND ENG CHEM RES. 2007;46:4914-4920*
Sudan crude oil	pilot-scale riser FCC unit; Y zeolite regenated FCC	T: 460°C; catalyst/oil: 5	Naphtha: 39.48wt%; Diesel: 29.88wt%	N/A	Two-stage FCC technology	*IND ENG CHEM RES. 2007;46:4914-4920*

	catalysts		LPG: 15.32wt%			
Daqing crude oil[a]	pilot-scale riser FCC unit; ZSM-5 zeolite	T: 530-590°C; catalyst/oil:10	**C_2-C_4 olefins yields: 31.37-33.48 wt%** Naphtha yields: 16.50-23.32wt%	0.51-0.59	COCC technology; Chemicals and fuels	UWs
Daqing crude oil[a]	pilot-scale riser FCC unit; ZSM-5 zeolite	T: 600-630°C; catalyst/oil:12	**C_2-C_4 olefins yields: 32.94-34.54 wt%** Naphtha yields: 14.50-17.29wt%	0.48-0.53	COCC technology; Chemicals and fuels	UWs
Daqing crude oil[a]	pilot-scale riser FCC unit; ZSM-5 zeolite	T: 650-690°C; catal/oil:15-20	**C_2-C_4 olefins yields: 36.13-40.46 wt%** Naphtha yields: 10.50-12.14wt%	0.36-0.40	COCC technology; Chemicals and fuels	UWs
Zhongyuan crude[a]	pilot-scale riser FCC unit; ZSM-5 zeolite	T: 650-690°C; catalyst/oil:15-20	**C_2-C_4 olefins yields: 33.28-37.12 wt%** Naphtha yields: 10.43-12.51wt%	0.41-0.46	COCC technology; Chemicals and fuels	UWs
Changqing crude[a]	pilot-scale riser FCC unit; ZSM-5 zeolite	T: 650-690°C; catalyst/oil: 15-20	**C_2-C_4 olefins yields: 32.34-37.69wt%** Naphtha yields: 10.90-13.87wt%	0.41-0.46	COCC technology; Chemicals and fuels	UWs

a: The pilot-test results of COCC technology using Daqing and Changqing crude oil by our research group are unpublished works (UWs)

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