

Supplementary Material for

Molecular Modelling of Co-processing Biomass

Fast Pyrolysis Oil in Fluid Catalytic Cracking Unit

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Table S1 Reactions and kinetic parameters for light gases (C1 to C4)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
1	C ₂ H ₄ + H ₂ → C ₂ H ₆	1.05959E-09	191	191
2	C ₃ H ₆ + H ₂ → C ₃ H ₈	3.44963E-09	340	340
3	nC ₄ H ₈ + H ₂ → nC ₄ H ₁₀	4.75375E-09	340	340
4	iC ₄ H ₈ + H ₂ → iC ₄ H ₁₀	5.12185E-09	340	340
5	C ₃ H ₆ + H ₂ → C ₂ H ₄ + CH ₄	3.15727E-09	211	211
6	nC ₄ H ₈ + H ₂ → C ₃ H ₆ + CH ₄	1.36196E-09	211	211
7	iC ₄ H ₈ + H ₂ → C ₃ H ₆ + CH ₄	3.31203E-09	211	211
8	C ₂ H ₆ → C ₂ H ₄ + H ₂	5.99478E-08	340	340
9	C ₃ H ₈ → C ₂ H ₄ + CH ₄	8.17224E-08	237	237
10	C ₃ H ₈ → C ₃ H ₆ + H ₂	6.09166E-09	227	227
11	nC ₄ H ₁₀ → C ₂ H ₄ + C ₂ H ₆	9.44624E-08	237	237
12	nC ₄ H ₁₀ → C ₃ H ₆ + CH ₄	1.09629E-07	227	227
13	nC ₄ H ₁₀ → 2C ₂ H ₄ + H ₂	9.15486E-07	305	305
14	nC ₄ H ₁₀ → C ₄ H ₈ + H ₂	4.81558E-07	207	207

15	iC_4H_{10}	\rightarrow	C_3H_6	+	CH_4	$7.55078E-07$	237	237		
16	iC_4H_{10}	\rightarrow	iC_4H_8	+	H_2	$5.66006E-07$	218	218		
17	nC_4H_8	\rightarrow	C_2H_4	+	C_2H_4	$4.26738E-07$	237	237		
18	C_2H_4	+	CH_4	\rightarrow	C_3H_6	+	H_2	$4.04041E-09$	204	204
19	C_3H_6	+	CH_4	\rightarrow	C_2H_4	+	C_2H_6	$5.81324E-09$	204	204
20	C_3H_6	+	CH_4	\rightarrow	C_4H_8	+	H_2	$7.91590E-09$	204	204
21	nC_4H_8	+	CH_4	\rightarrow	C_2H_4	+	C_3H_8	$3.03030E-09$	204	204
22	nC_4H_8	+	CH_4	\rightarrow	C_2H_6	+	C_3H_6	$5.84416E-09$	204	204
23	iC_4H_8	+	CH_4	\rightarrow	C_2H_4	+	C_3H_8	$8.68893E-09$	204	204
24	CH_4	+	CH_4	\rightarrow	C_2H_4	+	$2H_2$	0	204	204
25	C_2H_6	+	C_2H_4	\rightarrow	C_3H_6	+	CH_4	0	211	211

Table S2 Reactions and kinetic parameters for light gasoline paraffin lump (50-120°C)

Reaction Number	Reaction			Kinetic Parameter		
				k_0	Ea (this work)	Ea (Gomez- Prado ²⁰)
				[m ³ kg ⁻¹ s ⁻¹]	[kJ kmol ⁻¹]	[kJ kmol ⁻¹]
26	Pl	→	C1	3.745E-02	59576	63210
27	Pl	→	C2 -	4.601E-01	59576	63210
28	Pl	→	C2 =	5.599E-01	59576	63210
29	Pl	→	C3 -	1.161E+00	59576	63210
30	Pl	→	C3 =	1.774E+00	59576	63210
31	Pl	→	nC4 -	6.109E-01	59576	63210
32	Pl	→	iC4 -	2.829E-02	59576	63210
33	Pl	→	C4 =	1.885E+00	59576	63210
34	Pl	→	O1	1.010E+00	59576	72130

Table S3 Reactions and kinetic parameters for light gasoline olefin lump (50-120°C)

Reaction Number	Reaction				Kinetic Parameter			
					k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
35	H ₂	+	Ol	→	Pl	1.933E+11	109293	109293
36			Ol	→	Al	1.712E+04	127598	127598
37			Ol	→	C1	0.000E+00	31913	63210
38			Ol	→	C2 -	0.000E+00	31913	63210
39			Ol	→	C2 =	0.000E+00	31913	63210
40			Ol	→	C3 -	8.479E-01	31913	63210
41			Ol	→	C3 =	0.000E+00	31913	63210
42			Ol	→	nC4 -	0.000E+00	31913	63210
43			Ol	→	iC4 -	5.083E+00	31913	63210
44			Ol	→	C4 =	0.000E+00	31913	63210
45			Ol	→	Coke	0.000E+00	51554	49980
46	Ol	+	Al	→	Coke	3.403E-04	71636	54420

Table S4 Reactions and Kinetic Parameters for light gasoline Naphthene lump (50-120°C)

Reaction Number	Reaction				Kinetic Parameter				
					k_0	Ea (this work)	Ea (Gomez-Prado ²⁰)		
					[m ³ kg ⁻¹ s ⁻¹]	[kJ kmol ⁻¹]	[kJ kmol ⁻¹]		
47	H ₂	+	Nl	→	Pl		1.025E+00	57863	57863
48			Nl	→	Ol		2.180E+05	141248	141248
49			Nl	→	Al	+ H ₂	1.165E+16	316231	316231
50	Ol	+	Nl	→	Al	+ Pl	1.051E+02	79771	79771
51			Nl	→	C1		0.000E+00	31913	63210
52			Nl	→	C2 -		0.000E+00	31913	63210
53			Nl	→	C2 =		0.000E+00	31913	63210
54			Nl	→	C3 -		0.000E+00	31913	63210
55			Nl	→	C3 =		0.000E+00	31913	63210
56			Nl	→	nC4 -		5.198E-01	31913	63210
57			Nl	→	iC4 -		5.223E-02	31913	63210
58			Nl	→	C4 =		0.000E+00	31913	63210
59			Nl	→	Coke		7.486E-04	51554	49980

Table S5 Reactions and kinetic parameters for aromatic lump in light gasoline (50-120°C)

Reaction Number	Reaction			Kinetic Parameters		
				k_0	Ea (this work)	Ea (Gomez-Prado ²⁰)
				[m ³ kg ⁻¹ s ⁻¹]	[kJ kmol ⁻¹]	[kJ kmol ⁻¹]
60	Al	→	C1 -	7.643E-04	37620	37620
61	Al	→	C2 -	9.208E-05	37620	37620
62	Al	→	C2 =	8.289E-04	37620	37620
63	Al	→	C3 -	9.208E-06	37620	37620
64	Al	→	C3 =	1.541E-03	37620	37620
65	Al	→	nC4 -	1.392E-02	37620	37620
66	Al	→	iC4 -	7.902E-02	37620	37620
67	Al	→	C4 =	5.646E-02	37620	37620
68	Al	→	Coke	1.178E-01	71636	54420

Table S6 Reactions and kinetic parameters for paraffin lump in heavy gasoline (120-205°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
69	Ph → Ol + Gas	2.087E+01	47057	72130
70	Ph → Pl + Gas	6.301E+01	47057	72130
71	H ₂ + Ph → Pl	2.872E+03	47057	100982
72	Ph → nC4 -	4.657E-01	47057	63210
73	Ph → iC4 -	4.952E-01	47057	63210
74	Ph → C4 =	4.281E-01	47057	63210

Table S7 Reactions and kinetic parameters for olefin lump in heavy gasoline (120-205°C)

Reaction Number	Reaction						Kinetic Parameter			
							k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
75	H ₂	+	Oh	→	Pl	+	Gas	1.404E+01	71673	72130
76			Oh	→	Ol	+	Gas	5.121E+01	71673	72130
77	H ₂	+	Oh	→	Ph			7.949E+03	109293	109293
78			Oh	→	Ah			9.704E+04	127598	127598
79			Oh	→	nC4			4.178E-01	31913	63210
80			Oh	→	iC4 -			4.530E-01	31913	63210
81			Oh	→	C4 =			4.117E-01	31913	63210
82			Oh	→	Coke			2.884E-02	51554	49980
83	Ah	+	Oh	→	Coke			5.662E-02	71636	54420

Table S8 Reactions and kinetic parameters for heavy gasoline naphthene lump (120-205°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
84	Nh → NI + Gas	2.108E+02	71673	72130
85	H ₂ + Nh → Ph	2.760E+00	57863	57863
86	Nh → Oh	4.920E+05	141248	141248
87	Nh → Ah + H ₂	2.504E+16	316231	316231
88	Oh + Nh → Ah + Ph	4.080E+02	79771	79771
89	Nh → nC4 -	5.530E-01	31913	63210
90	Nh → iC4 -	6.354E-01	31913	63210
91	Nh → C4 =	5.971E-01	31913	63210
92	Nh → Coke	0.000E+00	51554	49980
93	NI + Nh → Coke	0.000E+00	51554	49980
94	Ah + Nh → Coke	1.750E-01	71636	54420
95	Al + Nh → Coke	1.344E-01	71636	54420

Table S9 Reactions and kinetic parameters for heavy gasoline aromatic lump (120-205°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
96	Ah → Al + Gas	9.874E+01	71673	72130
97	H ₂ + Ah → Pl	1.866E+29	500642	500642
98	Ah → Ol	2.893E+14	274508	274508
99	Ah → Coke	1.355E-01	71636	54420
100	Ol + Ah → Coke	0.000E+00	71636	54420
101	Al + Ah → Coke	1.123E-01	71636	54420

Table S10 Reactions and kinetic parameters for diesel paraffin lump (205-320°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
102	Pd → Pl + Oh	1.704E+00	122219	72130
103	Pd → Pl + Ol + Gas	1.459E+02	122219	72130
104	Pd → Ol + Ph	2.840E+01	122219	72130
105	Pd → Ph + Gas	7.305E+00	122219	72130
106	Pd → Nh	3.101E+03	122219	104589
107	Pd → Ah	1.169E+05	122219	127598
108	H ₂ + Pd → Pl	0.000E+00	122219	100982
109	Pd → iC4 -	2.085E+00	122219	63210
110	Pd → C4 =	6.393E+00	122219	63210
111	Pd → Coke	7.946E-03	122219	49980
112	Al + Pd → Coke	1.229E+00	122219	54420
113	Ah + Pd → Coke	1.747E+00	122219	54420

Table S11 Reactions and kinetic parameters for diesel olefin lump (205-320°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
114	H ₂ + Od → Ph + Gas	2.253E+01	71673	72130
115	Od → Oh + Gas	2.253E+01	71673	72130
116	H ₂ + Od → Pl	1.115E+04	109293	109293
117	Od → Ol	4.506E+01	71673	72130
118	H ₂ + Od → Pd	2.788E+03	109293	109293
119	Od → Ad	4.210E+04	127598	127598
120	Od → nC4 -	0.000E+00	31913	63210
121	Od → iC4 -	0.000E+00	31913	63210
122	Od → C4 =	0.000E+00	31913	63210
123	Od → Coke	1.266E+00	51554	49980
124	Ad + Od → Coke	2.445E+00	71636	54420

Table S12 Reactions and kinetic parameters for diesel naphthene lump (205-320°C)

Reaction Number	Reaction					Kinetic Parameter		
						k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
125	H ₂	+	Nd	→	Pd	1.903E-01	57863	57863
126			Nd	→	Od	0.000E+00	141248	141248
127			Nd	→	Ad + H ₂	4.190E+16	316231	316231
128			Nd	→	Nh + Gas	2.647E+01	71673	72130
129	H ₂	+	Nd	→	Nh + Pl	7.951E+00	71673	72130
130			Nd	→	Ah + Pl	4.469E-04	0	0
131			Nd	→	Nh + Ol	7.548E+00	71673	72130
132			Nd	→	Ah + Ol	0.000E+00	71673	72130
133	H ₂	+	Nd	→	Nl + Ph	4.246E+01	71673	72130
134			Nd	→	Nl + Oh	6.306E+00	71673	72130
135	H ₂	+	Nd	→	Oh + Pl	0.000E+00	58560	58560
136	H ₂	+	Nd	→	Ph + Ol	0.000E+00	58560	58560
137			Nd	→	Pl + Nl	2.181E-03	0	0
138			Nd	→	Ol + Nl	3.769E-04	0	0
139			Nd	→	Pl + Ol	2.818E-03	0	0
140	Od	+	Nd	→	Ad + Pd	6.180E+02	79771	79771
141			Nd	→	Coke	0.000E+00	51554	49980
142	Nl	+	Nd	→	Coke	0.000E+00	51554	49980
143	Nh	+	Nd	→	Coke	0.000E+00	51554	49980
144	Ah	+	Nd	→	Coke	0.000E+00	71636	54420
145	Al	+	Nd	→	Coke	0.000E+00	71636	54420
146	Ad	+	Nd	→	Coke	0.000E+00	71636	54420

Table S13 Reactions and kinetic parameters for diesel aromatic lump (205-320°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
147	H ₂ + Ad → Pl + Ah	3.406E+01	71673	72130
148	Ad → Ol + Ah	1.839E+01	71673	72130
149	Ad → Ah + Gas	1.499E+02	71673	72130
150	H ₂ + Ad → Ph + Al	9.432E+01	71673	72130
151	Ad → Oh + Al	4.298E+01	71673	72130
152	H ₂ + Ad → Pl + Al	1.592E+05	71673	72130
153	Ad → Ol + Al	7.707E+01	71673	72130
154	Ad → Coke	1.210E-01	71636	54420
155	Al + Ad → Coke	1.892E-01	71636	54420
156	Ah + Ad → Coke	1.668E-01	71636	54420
157	Ol + Ad → Coke	3.560E-01	71636	54420
158	Oh + Ad → Coke	6.103E-01	71636	54420

Table S14 Reactions and kinetic parameters for gasoil paraffin lump (320-500°C)

Reaction Number	Reaction					Kinetic Parameter		
						k_0	Ea (this work)	Ea (Gomez-Prado ²⁰)
						[m ³ kg ⁻¹ s ⁻¹]	[kJ kmol ⁻¹]	[kJ kmol ⁻¹]
159	Pm	→	Pd	+	Od	3.411E+02	74244	72130
160	Pm	→	Pd	+	Oh	1.492E+02	74244	72130
161	Pm	→	Od	+	Ph	1.492E+02	74244	72130
162	Pm	→	Om	+	Pl	1.385E+02	74244	72130
163	Pm	→	Pm	+	Ol	1.385E+02	74244	72130
164	Pm	→	Pm	+	Gas	5.647E+01	74244	72130
165	Pm	→	Om	+	Gas	5.647E+01	74244	72130
166	H ₂	+	Pm	→	Pd	7.922E+01	74244	100982
167			Pm	→	Nm	2.100E+02	74244	104589
168			Pm	→	Am	2.550E+02	74244	127598
169			Pm	→	Coke	0.000E+00	74244	49980
170	Al	+	Pm	→	Coke	8.250E-01	74244	54420
171	Ah	+	Pm	→	Coke	8.662E-01	74244	54420

Table S15 Reactions and kinetic parameters for gasoil olefin lump (320-500°C)

Reaction Number	Reaction						Kinetic Parameter			
							k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
172	H ₂	+	Om	→	Pm	+	Gas	4.497E+01	71673	72130
173			Om	→	Om	+	Gas	4.497E+01	71673	72130
174	H ₂	+	Om	→	Pm	+	Ol	1.102E+02	71673	72130
175	H ₂	+	Om	→	Om	+	Pl	1.102E+02	71673	72130
176	H ₂	+	Om	→	Pd	+	Oh	1.935E+02	71673	72130
177	H ₂	+	Om	→	Od	+	Ph	1.935E+02	71673	72130
178	H ₂	+	Om	→	Pm			1.586E+04	109293	109293
179			Om	→	Am			4.787E+05	127598	127598
180			Om	→	Coke			5.277E-01	51554	49980
181	Al	+	Om	→	Coke			1.112E+00	71636	54420
182	Ah	+	Om	→	Coke			1.205E+00	71636	54420
183	Ad	+	Om	→	Coke			1.297E+00	71636	54420
184	Am	+	Om	→	Coke			1.390E+00	71636	54420

Table S16 Reactions and kinetic parameters for gasoil naphthene lump (320-500°C)

Reaction Number	Reaction			Kinetic Parameter				
				k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]		
185	H ₂	+	Nm → Pm	3.015E+01	57863	57863		
186			Nm → Om	3.032E+06	141248	141248		
187			Nm → Am	+	H ₂	3.690E+18	316231	316231
188			Nm → Nm	+	Gas	8.614E+01	71673	72130
189			Nm → Nm	+	Pl	9.923E+01	71673	72130
190			Nm → Nm	+	Ol	9.923E+01	71673	72130
191	H ₂	+	Nm → Nd	+	Ph	1.508E+02	71673	72130
192			Nm → Nd	+	Oh	1.508E+02	71673	72130
193	H ₂	+	Nm → Nh	+	Pd	1.330E+02	71673	72130
194			Nm → Nh	+	Od	1.330E+02	71673	72130
195	H ₂	+	Nm → Nl	+	Pd	1.231E+02	71673	72130
196			Nm → Nl	+	Od	1.231E+02	71673	72130
197	Om	+	Nm → Am	+	Pm	8.926E+03	79771	79771
198			Nm → Coke			5.039E-01	51554	49980
199	Nl	+	Nm → Coke			2.230E-01	51554	49980
200	Nh	+	Nm → Coke			2.972E-01	51554	49980
201	Nd	+	Nm → Coke			3.716E-01	51554	49980
202	Al	+	Nm → Coke			2.872E-01	71636	54420
203	Ah	+	Nm → Coke			5.742E-01	71636	54420
204	Ad	+	Nm → Coke			8.614E-01	71636	54420
205	Am	+	Nm → Coke			1.149E+00	71636	54420

Table S17 Reactions and kinetic parameters for gasoil aromatic lump (320-500°C)

Reaction Number	Reaction						Kinetic Parameter			
							k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
206	H ₂	+	Am	→	Al	+	Pm	5.368E+01	71673	72130
207			Am	→	Al	+	Om	5.368E+01	71673	72130
208	H ₂	+	Am	→	Ah	+	Pd	5.780E+01	71673	72130
209			Am	→	Ah	+	Od	5.780E+01	71673	72130
210	H ₂	+	Am	→	Ad	+	Ph	6.514E+01	71673	72130
211			Am	→	Ad	+	Oh	6.514E+01	71673	72130
212	H ₂	+	Am	→	Am	+	Pl	4.572E+01	71673	72130
213			Am	→	Am	+	Ol	4.572E+01	71673	72130
214			Am	→	Am	+	Gas	4.846E+01	71673	72130
215			Am	→	Coke			1.951E+00	71636	54420
216	Al	+	Am	→	Coke			7.802E-01	71636	54420
217	Ah	+	Am	→	Coke			1.951E-01	71636	54420
218	Ad	+	Am	→	Coke			3.902E-02	71636	54420
219	Oh	+	Am	→	Coke			3.308E-02	71636	54420
220	Ol	+	Am	→	Coke			1.653E-02	71636	54420
221	Od	+	Am	→	Coke			6.612E-02	71636	54420

Table S18 Reactions and kinetic parameters for residue paraffins lump (> 500°C)

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
222	Pr → Pm + Om	7.849E+02	77331	72130
223	Pr → Pm + Od	3.321E+02	77331	72130
224	Pr → Om + Pd	3.321E+02	77331	72130
225	Pr → Or + Ph	3.019E+02	77331	72130
226	Pr → Pr + Oh	3.019E+02	77331	72130
227	Pr → Or + Pl	2.868E+02	77331	72130
228	Pr → Pr + Ol	2.868E+02	77331	72130
229	Pr → Or + Gas	1.540E+02	77331	72130
230	Pr → Pr + Gas	1.540E+02	77331	72130
231	H ₂ + Pr → Pm	2.266E+03	77331	100982
232	Pr → Nr	4.760E+02	77331	104589
233	Pr → Ar	5.696E+02	77331	127598
234	Pr → Coke	9.395E-01	77331	49980
235	Al + Pr → Coke	1.966E+00	77331	54420
236	Ah + Pr → Coke	2.184E+00	77331	54420
237	Ad + Pr → Coke	2.402E+00	77331	54420
238	Am + Pr → Coke	2.621E+00	77331	54420

Table S19 Reactions and kinetic parameters for residue olefin lump (> 500°C)

Reaction Number	Reaction						Kinetic Parameter			
							k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
239	H ₂	+	Or	→	Pr	+	Gas	1.148E+02	71673	72130
240			Or	→	Or	+	Gas	1.148E+02	71673	72130
241	H ₂	+	Or	→	Pr	+	Ol	2.129E+02	71673	72130
242			Or	→	Or	+	Pl	2.129E+02	71673	72130
243	H ₂	+	Or	→	Pm	+	Oh	4.802E+02	71673	72130
244	H ₂	+	Or	→	Om	+	Ph	4.802E+02	71673	72130
245	H ₂	+	Or	→	Pd	+	Od	5.744E+02	71673	72130
246	H ₂	+	Or	→	Pr			4.084E+04	109293	109293
247			Or	→	Ar			1.233E+06	127598	127598
248			Or	→	Coke			1.086E+00	51554	49980
249	Al	+	Or	→	Coke			9.548E-01	71636	54420
250	Ah	+	Or	→	Coke			2.387E-01	71636	54420
251	Ad	+	Or	→	Coke			1.432E+00	71636	54420
252	A m	+	Or	→	Coke			1.910E+00	71636	54420
253	Ar	+	Or	→	Coke			2.387E+00	71636	54420

Table S20 Reactions and kinetic parameters for residue naphthene lump (> 500°C)

Reaction Number	Reaction					Kinetic Parameter		
						k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]
254	Ad	+	Nr	→	Coke	2.212E+00	71636	54420
255	Am	+	Nr	→	Coke	3.538E+00	71636	54420
256	Ar	+	Nr	→	Coke	3.982E+00	71636	54420
257	H ₂	+	Nr	→	Pr	7.889E+01	57863	57863
258			Nr	→	Or	7.957E+06	141248	141248
259			Nr	→	Ar + H ₂	9.662E+18	316231	316231
260			Nr	→	Nr + Gas	1.223E+02	71673	72130
261	H ₂	+	Nr	→	Nr + Pl	1.834E+02	71673	72130
262			Nr	→	Nr + Ol	1.834E+02	71673	72130
263	H ₂	+	Nr	→	Nm + Ph	4.188E+02	71673	72130
264			Nr	→	Nm + Oh	4.188E+02	71673	72130
265	H ₂	+	Nr	→	Nd + Pd	3.699E+02	71673	72130
266			Nr	→	Nd + Od	3.699E+02	71673	72130
267	H ₂	+	Nr	→	Nh + Pm	3.455E+02	71673	72130
268			Nr	→	Nh + Om	3.455E+02	71673	72130
269	H ₂	+	Nr	→	Nl + Pr	3.210E+02	71673	72130
270			Nr	→	Nl + Or	3.210E+02	71673	72130
271	Or	+	Nr	→	Ar + Pr	1.167E+04	79771	79771
272			Nr	→	Coke	1.397E+00	51554	49980
273	Nl	+	Nr	→	Coke	2.290E-01	51554	49980
274	Nh	+	Nr	→	Coke	4.580E-01	51554	49980
275	Nd	+	Nr	→	Coke	6.868E-01	51554	49980
276	Nm	+	Nr	→	Coke	1.145E+00	51554	49980
277	Al	+	Nr	→	Coke	1.327E+00	71636	54420
278	Ah	+	Nr	→	Coke	1.769E+00	71636	54420

Table S21 Reactions and kinetic parameters for residue aromatic lump (> 500°C)

Reaction Number	Reaction						Kinetic Parameter			
							k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Gomez-Prado ²⁰) [kJ kmol ⁻¹]	
279	H ₂	+	Ar	→	Al	+	Pr	6.545E+01	71673	72130
280			Ar	→	Al	+	Or	6.545E+01	71673	72130
281	H ₂	+	Ar	→	Ah	+	Pm	6.969E+01	71673	72130
282			Ar	→	Ah	+	Om	6.969E+01	71673	72130
283	H ₂	+	Ar	→	Ad	+	Pd	7.539E+01	71673	72130
284			Ar	→	Ad	+	Od	7.539E+01	71673	72130
285	H ₂	+	Ar	→	Am	+	Ph	8.442E+01	71673	72130
286			Ar	→	Am	+	Oh	8.442E+01	71673	72130
287	H ₂	+	Ar	→	Ar	+	Pl	4.740E+01	71673	72130
288			Ar	→	Ar	+	Ol	4.740E+01	71673	72130
289			Ar	→	Ar	+	Gas	2.845E+01	71673	72130
290			Ar	→	Coke			1.441E+01	71636	54420
291	Al	+	Ar	→	Coke			4.801E+00	71636	54420
292	Ah	+	Ar	→	Coke			6.861E+00	71636	54420
293	Ad	+	Ar	→	Coke			8.918E+00	71636	54420
294	Am	+	Ar	→	Coke			1.028E+01	71636	54420
295	Ol	+	Ar	→	Coke			6.861E-01	71636	54420
296	Oh	+	Ar	→	Coke			2.744E+00	71636	54420
297	Od	+	Ar	→	Coke			4.801E+00	71636	54420
298	Om	+	Ar	→	Coke			6.861E+00	71636	54420

Table S22 Reactions and kinetic parameters for carboxylic acids and esters (ES) lump

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Adjaye and Bakhshi ³⁷) [kJ kmol ⁻¹]
322	Alcohol(l) → C2- + CO	2.100E-01	5264	37000
323	Alcohol(h) → C3- + CO	2.100E-01	5264	37000
324	Alcohol(l) → C2 = + H ₂ O	2.100E-01	5264	37000
325	Alcohol(h) → Ol + H ₂ O	2.100E-03	5930	6700
326	Alcohol(d) → Oh + H ₂ O	2.100E-03	5930	6700
327	Alcohol(m) → Od + H ₂ O	2.100E-03	5930	6700
328	Alcohol(m) → Om + H ₂ O	2.100E-03	5930	6700

Table S23 Reactions and kinetic parameters for phenolics (Phe) lump

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Adjaye and Bakhshi ³⁷) [kJ kmol ⁻¹]
305	Phe(l) + H ₂ → A(l) + H ₂ O	2.100E-03	5930	6700
306	Phe(h) + H ₂ → A(l) + H ₂ O	2.100E-03	5930	6700
307	Phe(d) + H ₂ → A(h) + H ₂ O	2.100E-03	5930	6700
308	Phe(m) + H ₂ → A(d) + H ₂ O	2.100E-03	5930	6700
309	Phe(r) + H ₂ → A(m) + H ₂ O	2.100E-03	5930	6700
310	Phe(LG) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000
311	Phe(l) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000
312	Phe(h) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000
313	Phe(d) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000
314	Phe(m) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000
315	Phe(r) + H ₂ → Coke + H ₂ O	3.310E+01	92508	73000

Table S24 Reactions and kinetic parameters for aldehydes and ketones lump

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Adjaye and Bakhshi ³⁷) [kJ kmol ⁻¹]
316	Ald & Ket (LG) + H ₂ → C3 = + H ₂ O	1.200E-01	92508	37000
317	Ald & Ket (l) + H ₂ → nC4 + H ₂ O	1.200E-01	92508	37000
318	Ald & Ket (h) + H ₂ → Ol + H ₂ O	2.100E-03	5930	6700
319	Ald & Ket (d) + H ₂ → Oh + H ₂ O	2.100E-03	5930	6700
320	Ald & Ket (m) + H ₂ → Od + H ₂ O	2.100E-03	5930	6700
321	Ald & Ket (r) + H ₂ → Om + H ₂ O	2.100E-03	5930	6700

Table S25 Reactions and kinetic parameters for alcohol lump

Reaction Number	Reaction	Kinetic Parameter		
		k_0 [m ³ kg ⁻¹ s ⁻¹]	Ea (this work) [kJ kmol ⁻¹]	Ea (Adjaye and Bakhshi ³⁷) [kJ kmol ⁻¹]
322	Alcohol (l) → C2- + CO	2.100E-01	5264	37000
323	Alcohol (h) → C3- + CO	2.100E-01	5264	37000
324	Alcohol (l) → C2 = + H ₂ O	2.100E-01	5264	37000
325	Alcohol (h) → Ol + H ₂ O	2.100E-03	5930	6700
326	Alcohol (d) → Oh + H ₂ O	2.100E-03	5930	6700
327	Alcohol (m) → Od + H ₂ O	2.100E-03	5930	6700
328	Alcohol (m) → Om + H ₂ O	2.100E-03	5930	6700