Supporting Information

Thermogravimetric pyrolysis behavior and kinetic study of two different organic-rich mudstones via multiple kinetic methods

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Supplementary Tables and Figures

Tables

Table S1. Calculation results of the activation energy and reaction mechanism of MP using Coats-Redfern method.

Model	5 K/min		10 K/min		20 K/min		40 K/min		Average E	Average R^2
	E	R^2	E	R^2	E	R^2	E	R^2		
F1	125.56	0.95608	138.18	0.94507	137.35	0.93584	139.84	0.92974	135.23	0.94168
F2	187.05	0.98380	208.74	0.98047	209.06	0.97857	212.01	0.97575	204.21	0.97965
F3	265.15	0.97997	298.46	0.9817	299.28	0.98311	304.310	0.98317	291.80	0.98199
F4	352.09	0.96890	398.41	0.97372	400.93	0.97703	406.67	0.97832	389.53	0.97449
P2	36.66	0.85161	39.93	0.82731	39.57	0.80936	40.07	0.79261	39.06	0.82022
R2	102.68	0.92536	111.95	0.90887	111.80	0.89892	113.51	0.88869	109.99	0.90546
D1	182.06	0.90058	197.53	0.88284	195.46	0.86862	198.73	0.8574	193.44	0.87736
D2	202.60	0.91997	244.16	0.93361	219.17	0.8926	222.65	0.88241	222.15	0.90715
D-ZLT3	299.19	0.97296	330.39	0.96523	330.66	0.96061	334.41	0.95464	323.66	0.96336
A1/2	262.64	0.96028	288.52	0.94981	288.48	0.94341	291.99	0.93572	282.91	0.94731
A2/3	193.95	0.95888	213.76	0.94865	212.94	0.94117	215.94	0.93394	209.15	0.94566
F1(0.05-0.75)	154.86	0.99143	179.70	0.99397	185.84	0.99542	194.85	0.99635	178.81	0.99429
A2/3(0.05-0.75)	237.98	0.99271	256.37	0.99701	284.84	0.9965	298.21	0.99732	269.35	0.99589

A5/6(0.05-0.75)	190.38	0.99312	219.16	0.99534	227.26	0.99672	233.99	0.99763	218.85	0.99570
F3(0.75-0.95)	214.47	0.98806	223.74	0.97833	219.70	0.98171	215.99	0.98202	218.47	0.98253

Table S2. Calculation results of the activation energy and reaction mechanism of UC (Peak I) using Coats-Redfern method.

Model	5 K/min		10 K/min		20 K/min		40 K/min		Average E	Average R^2
	E	R^2	E	R^2	E	R^2	E	R^2		
F1	127.30	0.99639	128.50	0.99585	126.85	0.99341	129.33	0.99444	128.00	0.99502
F2	181.71	0.98573	184.48	0.98684	183.63	0.99099	186.94	0.98984	184.19	0.98835
F3	250.13	0.95346	254.49	0.95531	255.04	0.96372	259.85	0.96133	254.88	0.95846
P2	39.23	0.94816	39.30	0.94334	38.15	0.92862	38.86	0.93232	38.88	0.93811
R2	106.65	0.98417	107.39	0.98231	105.33	0.97551	107.65	0.97815	106.75	0.98004
D1	191.74	0.96592	192.820	0.96307	189.24	0.95419	193.12	0.95713	191.73	0.96008
D2	211.59	0.97870	212.960	0.9765	209.16	0.96925	213.84	0.9721	211.89	0.97414
D-ZLT3	298.81	0.99770	302.33	0.99786	299.74	0.99793	305.64	0.99814	301.63	0.99791
A1/2	266.33	0.99677	268.90	0.99629	266.05	0.99417	271.01	0.99499	268.07	0.99556
A2/3	196.77	0.99663	198.77	0.99617	196.49	0.99396	200.30	0.9949	198.08	0.99542
A1/2 (0.05-0.2)	248.08	0.99970	254.00	0.99975	261.28	0.99977	266.16	0.99988	257.38	0.99978
A2/3 (0.05-0.2)	183.31	0.99970	187.70	0.99975	193.09	0.99976	196.69	0.99987	190.20	0.99977

A1/2 (0.2-0.7)	297.66	0.99991	300.66	0.99992	300.06	0.99983	302.80	0.99992	300.29	0.99990
A2/3 (0.2-0.7)	220.32	0.99990	222.50	0.99992	221.97	0.99982	223.98	0.99991	222.20	0.99989
A4/5 (0.2-0.7)	181.63	0.99990	183.43	0.99991	182.96	0.99982	184.59	0.99991	183.15	0.99989
F2 (0.7-0.95)	224.99	0.99978	223.50	0.99946	207.88	0.99921	215.98	0.99884	218.09	0.99932

Table S3. Calculation results of the activation energy and reaction mechanism of UC (Peak II) using Coats-Redfern method.

Model	5 K/min		10 K/min		20 K/min		40 K/min		Average E	Average R^2
	E	R^2	E	R^2	E	R^2	E	R^2		
F1	128.00	0.96746	120.37	0.95464	119.73	0.95785	110.82	0.94651	119.73	0.95662
F2	185.43	0.99343	177.85	0.99064	177.29	0.99068	166.31	0.98694	176.72	0.99042
F3	256.88	0.98118	250.14	0.98308	249.36	0.9809	236.56	0.98028	248.24	0.98136
P2	37.41	0.84165	33.61	0.79651	33.06	0.79838	29.24	0.75543	33.33	0.79799
R2	105.81	0.93080	98.17	0.91024	97.64	0.9145	89.76	0.89657	97.84	0.91303
D1	189.63	0.89650	174.59	0.87155	174.13	0.87663	160.09	0.85652	174.61	0.87530
D2	211.06	0.92301	195.98	0.90248	195.47	0.90695	180.35	0.89063	195.72	0.90577
D-ZLT3	303.61	0.98441	288.45	0.97685	287.49	0.97917	269.06	0.97183	287.15	0.97807
A2/3	198.53	0.96973	187.31	0.95801	186.43	0.96126	173.26	0.95120	186.38	0.96005
F1 (0.05-0.34)	203.70	0.99582	217.50	0.99209	213.80	0.98855	220.81	0.98210	213.95	0.98964

A2 (0.05-0.34)	95.58	0.99520	102.46	0.99100	100.34	0.98692	103.69	0.97962	100.52	0.98819
A1.5 (0.05-0.34)	131.82	0.99544	141.34	0.99314	138.49	0.98758	143.30	0.98056	138.74	0.98918
F2 (0.34-0.78)	157.39	0.99972	148.23	0.99967	148.74	0.99979	136.43	0.99962	147.70	0.99970
F1 (0.78-0.95)	106.60	0.99357	89.92	0.99635	98.27	0.99248	91.59	0.99158	96.60	0.99350
A2/3 (0.78-0.95)	166.59	0.99416	141.83	0.99674	154.84	0.99315	144.94	0.9925	152.05	0.99414
A3/4 (0.78-0.95)	147.50	0.99351	132.56	0.9935	136.12	0.99293	127.97	0.99172	136.04	0.99292

Table S4. The linear equation of E and InA and kinetic parameters at different heating rates.

Sample	Heating rate	Equation	R^2	Initial A
MP	5	InA=0.169E−3.612	0.98689	1.41×10^{12} (0.05-0.75) 5.18×10^{13} (0.75-0.95)
	10	InA=0.166E−2.968	0.98992	1.43×10^{12} (0.05-0.75) 4.89×10^{13} (0.75-0.95)
	20	InA=0.162E−2.349	0.98849	1.46×10^{12} (0.05-0.75) 4.72×10^{13} (0.75-0.95)
	40	InA=0.159E−1.694	0.98815	1.45×10^{12} (0.05-0.75) 4.31×10^{13} (0.75-0.95)
UC-Peak I	5	InA=0.170E−3.176	0.98801	9.21×10^{11} (0.05-0.2) 3.33×10^{12} (0.2-0.7) 2.33×10^{12} (0.7-0.95)
	10	InA=0.167E−2.552	0.98778	9.77×10^{11} (0.05-0.2) 3.45×10^{12} (0.2-0.7) 2.43×10^{12} (0.7-0.95)
	20	InA=0.167E−1.983	0.98705	9.24×10^{11} (0.05-0.2) 3.12×10^{12} (0.2-0.7) 2.22×10^{12} (0.7-0.95)
	40	InA=0.160E−1.305	0.98704	9.88×10^{11} (0.05-0.2) 3.31×10^{12} (0.2-0.7) 2.37×10^{12} (0.7-0.95)
UC-Peak II	5	InA=0.150E−2.848	0.98590	3.69×10^{8} (0.05-0.34) 1.50×10^{8} (0.34-0.78) 2.42×10^{7} (0.78-0.95)
	10	InA=0.149E−2.878	0.98387	3.79×10^{8} (0.05-0.34) 1.54×10^{8} (0.34-0.78) 2.50×10^{7} (0.78-0.95)
	20	InA=0.145E−2.270	0.98559	3.18×10^{8} (0.05-0.34) 1.32×10^{8} (0.34-0.78) 2.27×10^{7} (0.78-0.95)
	40	InA=0.144E−1.922	0.97999	4.09×10^{8} (0.05-0.34) 1.71×10^{8} (0.34-0.78) 2.96×10^{7} (0.78-0.95)

Table S5. The final pre-exponential factors A and the correlation coefficients R^2 between experimental data and simulated data of MP.

Heating rate	α∈(0-0.75)		α∈(0.75-1)	
	A	R_2	A	R_2
5 K/min	5.28×10^{12}	0.99134	2.52×10^{15}	0.91767
10 K/min	5.35×10^{12}	0.98632	2.38×10^{15}	0.94258
20 K/min	5.53×10^{12}	0.98453	2.30×10^{15}	0.92736
40 K/min	5.45×10^{12}	0.97775	2.10×10^{15}	0.91650
Average	5.40×10^{12}	0.98499	2.32×10^{15}	0.92603

Table S6. The final pre-exponential factors A and the correlation coefficients R^2 between experimental data and simulated data of UC-Peak I.

Heating	α∈(0-0.2)		α∈(0.2-0.7)		α∈(0.7-1)	
rate	A	R_2	A	R_2	A	R_2
5	9.76×10^{11}	0.98908	6.36×10^{12}	0.96828	9.07×10^{12}	0.98876
10	1.04×10^{12}	0.98679	6.60×10^{12}	0.97320	9.46×10^{12}	0.98386
20	9.79×10^{11}	0.98540	5.97×10^{12}	0.93161	8.63×10^{12}	0.97015
40	1.05×10^{12}	0.98693	6.33×10^{12}	0.96736	9.21×10^{12}	0.97357
Average	1.01×10^{12}	0.98705	6.32×10^{12}	0.96011	9.09×10^{12}	0.97909

Table S7. The final pre-exponential factors A and the correlation coefficients R^2 between experimental data and simulated data of UC-Peak II.

Heating rate	α∈(0-0.34)		α∈(0.34-0.78)		α∈(0.78-1)	
	A	R_2	A	R_2	A	R_2
5	8.18×10^8	0.97582	7.37×10^7	0.98945	9.61×10^5	0.98686
10	8.38×10^8	0.98135	7.58×10^7	0.98410	9.94×10^5	0.96343
20	7.03×10^8	0.98362	6.52×10^7	0.99004	9.02×10^5	0.97204
40	9.06×10^8	0.94376	8.44×10^7	0.93584	1.18×10^6	0.93998
Average	8.16×10^8	0.97114	7.48×10^7	0.97486	1.01×10^6	0.93998

Figures

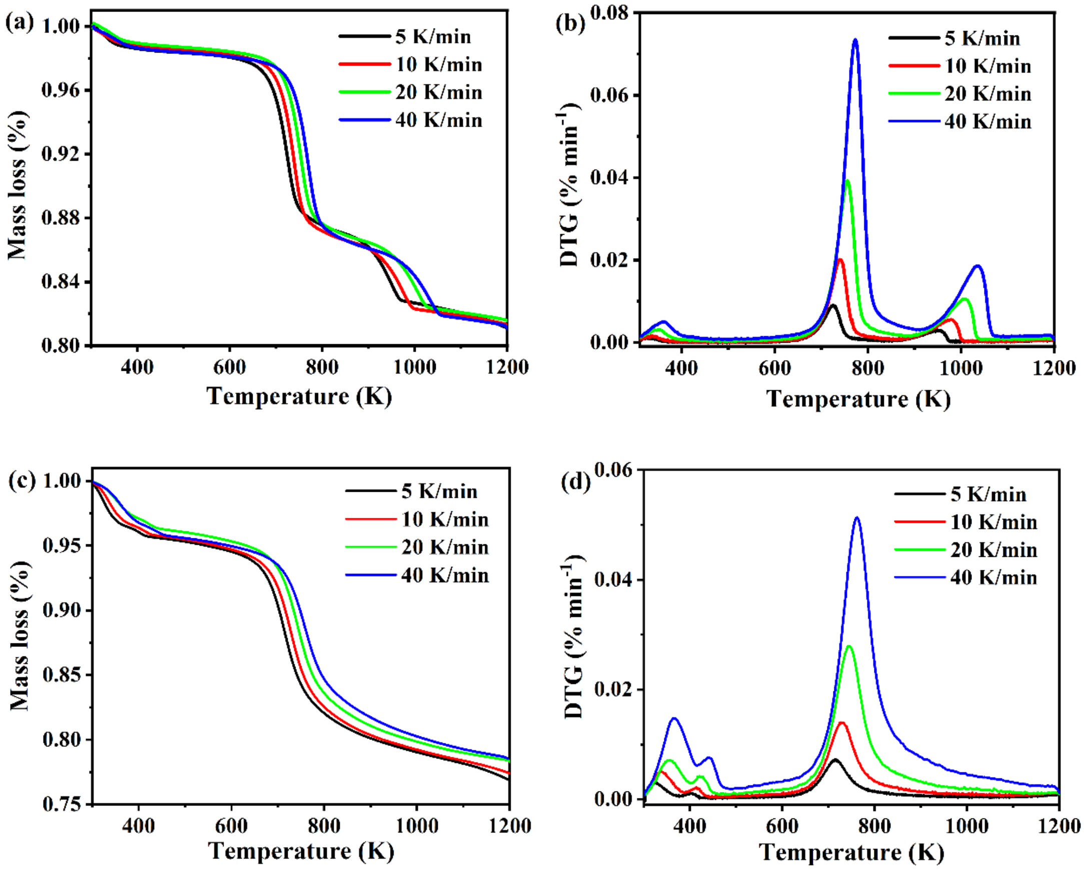

Figure S1. TG and DTG curves of (a, b) MP; (c, d) UC.

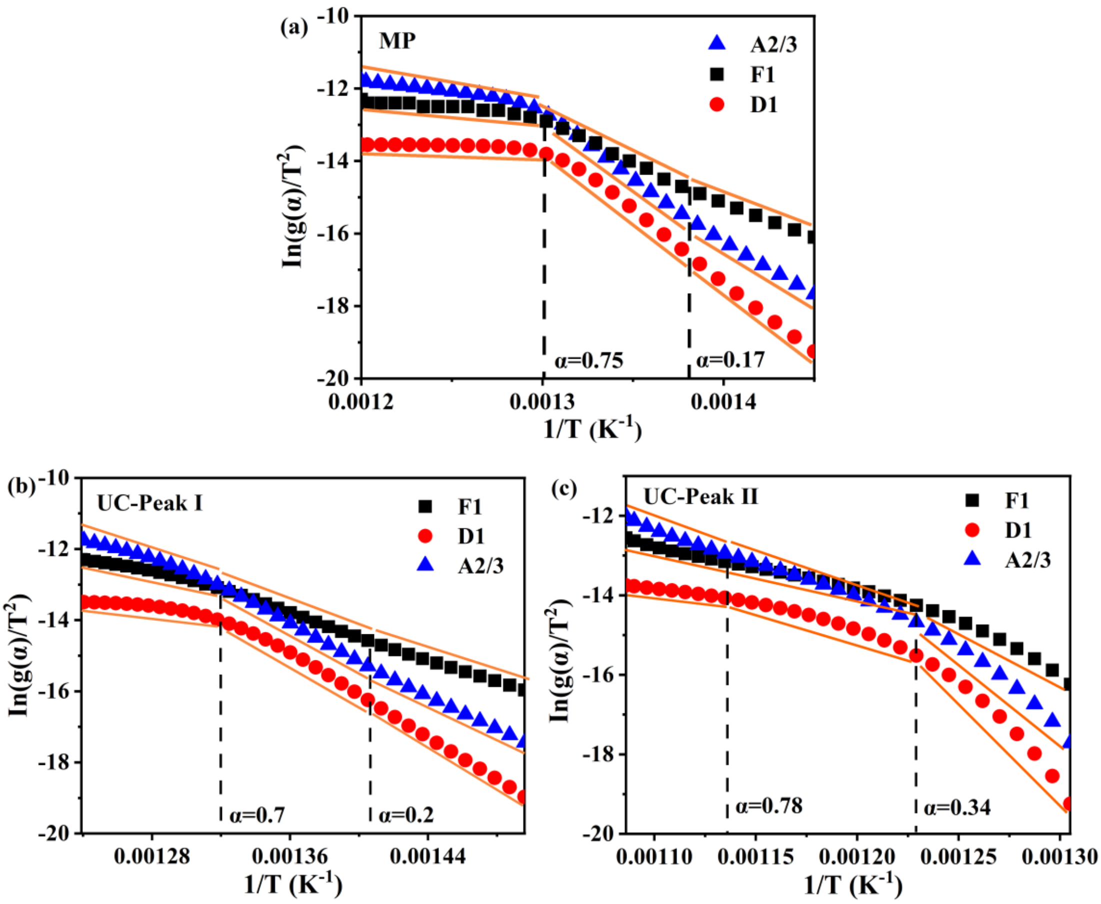

Figure S2. The plot of $\ln(g(\alpha)/T^2)$ against 1/T when the reaction model is F_1, D_1 and $A_{2/3}$ at 20 K/min for (a) MP; (b) UC-Peak I; (c) UC-Peak II.