Supplementary file

Occurrence states of organic matter modulate the surface properties of shale nanopores

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Appendix A: Supplementary data

Table S1. Sample information and the pyrolysis characteristics of raw, extracted and oxidized samples.

No.	Well	Depth	Formation	Raw					Extracted			Oxidized		
				S_1 (mg/g)	S_2 (mg/g)	TOC (%)	T_{max} (℃)	HI (mg/g)	S_1 (mg/g)	S_2 (mg/g)	TOC (%)	S_1 (mg/g)	S_2 (mg/g)	TOC (%)
1	NY1	3300.90	Es_3^{lower}	3.03	25.58	4.45	442	575	0.04	23.18	3.98	0.38	17.17	3.99
2	NY1	3315.10	Es_3^{lower}	2.61	16.58	3.08	441	538	0.03	9.76	2.16	0.23	7.55	2.36
3	NY1	3326.85	Es_4^{upper}	1.60	8.48	1.69	440	502	0.05	5.57	1.35	0.17	3.33	1.17
4	NY1	3344.66	Es_4^{upper}	2.29	10.71	2.30	441	466	0.03	6.47	1.58	0.18	3.12	1.50
5	NY1	3354.41	Es_4^{upper}	1.98	10.29	2.11	443	488	0.14	8.22	1.67	0.19	4.40	1.73
6	NY1	3369.91	Es_4^{upper}	2.86	9.58	2.14	442	448	0.03	5.70	1.44	0.16	2.83	1.50
7	NY1	3383.81	Es_4^{upper}	2.59	9.48	1.85	443	512	0.02	4.54	1.11	0.20	3.63	1.38
8	NY1	3396.75	Es_4^{upper}	6.86	25.15	5.13	442	490	0.08	14.01	3.41	0.31	7.66	3.03
9	NY1	3413.84	Es_4^{upper}	7.89	35.59	5.56	449	640	0.05	23.41	3.97	0.48	19.63	3.78
10	NY1	3429.23	Es_4^{upper}	3.85	13.37	2.47	442	541	0.03	8.55	1.47	0.21	6.14	1.32
11	NY1	3432.73	Es_4^{upper}	5.66	32.26	5.56	448	580	0.07	23.59	3.98	0.44	19.19	3.72
12	NY1	3452.16	Es_4^{upper}	2.64	6.79	1.79	439	379	0.02	2.60	1.00	0.11	1.73	0.72
13	NY1	3465.03	Es_4^{upper}	2.59	9.28	2.33	438	398	0.08	4.87	1.47	0.14	2.39	1.12
14	NY1	3482.38	Es_4^{upper}	3.43	5.19	1.82	432	285	0.04	0.96	0.94	0.08	0.50	0.97
15	N876	3372.50	Es_3^{lower}	1.45	30.8	5.14	441	599	0.39	25.91	4.63	0.36	18.42	4.69
16	N876	3376.40	Es_3^{lower}	1.06	13.09	2.42	442	541	0.27	10.12	2.17	0.24	7.43	2.09
17	N876	3377.30	Es_3^{lower}	5.12	49.03	7.52	440	652	0.50	38.51	6.23	0.57	26.68	6.24
18	N876	3378.20	Es_3^{lower}	0.68	4.46	1.24	437	360	0.12	2.83	0.93	0.11	1.73	0.91
19	N876	3397.70	Es_3^{lower}	6.53	73.24	10.87	441	674	0.60	60.56	8.82	0.53	42.81	9.24
20	LY1	3593.30	Es_3^{lower}	8.38	19.43	4.81	444	404	0.38	9.44	3.23	0.32	6.43	2.94
21	LY1	3602.60	Es_3^{lower}	5.41	12.90	3.50	446	369	0.28	6.65	2.45	0.26	4.34	2.15
22	LY1	3616.90	Es_3^{lower}	7.23	13.74	3.83	444	359	0.40	7.14	2.59	0.27	4.91	2.29
23	LY1	3634.20	Es_3^{lower}	6.32	12.47	3.30	436	378	0.26	4.58	1.92	0.17	1.82	1.25
24	LY1	3641.80	Es_3^{lower}	6.73	11.03	2.88	436	383	0.30	3.72	1.50	0.18	1.54	1.17
25	LY1	3658.52	Es_3^{lower}	13.65	26.11	7.68	447	340	0.78	16.49	5.55	0.42	9.73	4.90
26	LY1	3676.27	Es_3^{lower}	3.73	7.33	2.30	437	319	0.21	2.15	1.65	0.11	0.67	0.68
27	LY1	3690.70	Es_3^{lower}	2.72	5.04	1.69	438	298	0.22	1.71	1.21	0.09	0.48	0.75
28	LY1	3736.50	Es_4^{upper}	4.08	7.36	2.44	432	302	0.28	2.44	1.77	0.12	0.89	0.85
29	LY1	3752.90	Es_4^{upper}	2.42	4.42	1.72	432	257	0.27	1.59	1.38	0.08	0.37	0.78
30	LY1	3768.20	Es_4^{upper}	5.08	7.71	2.62	433	294	0.37	2.58	1.87	0.13	0.80	0.75
31	LY1	3775.60	Es_4^{upper}	6.76	10.59	3.68	428	288	0.30	2.85	2.52	0.14	1.04	1.13
32	LY1	3792.40	Es_4^{upper}	4.78	6.80	2.49	434	273	0.26	2.26	1.87	0.14	0.76	1.21
33	LY1	3800.52	Es_4^{upper}	9.97	13.9	5.63	444	247	0.46	5.20	4.53	0.27	2.29	3.12
34	LY1	3809.80	Es_4^{upper}	6.95	8.05	3.03	444	266	0.25	3.28	2.12	0.27	1.47	1.11
35	LY1	3816.50	Es_4^{upper}	6.21	6.91	2.48	420	279	0.24	1.34	1.60	0.20	0.51	0.97
36	LS101	4134.20	Es_4^{upper}	1.69	4.56	3.81	460	120	0.48	3.03	3.89	0.18	0.91	2.22
37	LS101	4165.00	Es_4^{upper}	1.02	2.57	2.94	462	87	0.34	2.10	2.84	0.08	0.28	0.86
38	LS101	4166.90	Es_4^{upper}	1.31	3.97	4.10	464	97	0.48	3.22	4.32	0.15	0.70	1.77
39	LS101	4168.30	Es_4^{upper}	1.15	2.85	2.01	458	142	0.44	1.52	1.91	0.08	0.18	0.35
40	LS101	4170.10	Es_4^{upper}	0.99	1.39	1.41	462	99	0.38	0.68	1.32	0.03	0.09	0.21
41	LS101	4172.00	Es_4^{upper}	0.78	1.41	1.94	456	73	0.37	1.09	1.97	0.08	0.28	0.86
42	LS101	4288.70	Es_4^{upper}	1.20	2.56	2.90	464	88	0.38	2.12	2.93	0.11	0.50	1.29
43	LS101	4329.00	Es_4^{upper}	1.71	2.88	3.53	464	82	0.48	2.48	3.61	0.27	0.69	1.83

Table S2. Changes of the SSA achieved by N_2 adsorption before and after pretreatments.

No.	SSA (m^2/g)			No.	SSA (m^2/g)			No.	SSA (m^2/g)		
	Raw	Extracted	Oxidized		Raw	Extracted	Oxidized		Raw	Extracted	Oxidized
1	0.11	8.55	11.38	16	1.95	19.87	22.49	30	4.13	18.39	18.76
2	1.64	19.77	25.56	17	2.17	15.49	15.65	31	3.71	24.13	28.53
3	0.89	22.70	28.25	18	22.98	39.55	39.97	32	3.30	15.40	16.69
4	2.14	16.99	23.96	19	0.83	6.21	6.95	33	4.17	21.41	20.68
5	0.25	10.08	13.02	20	1.72	5.59	5.66	34	2.00	10.24	8.65
6	2.13	17.98	24.54	21	1.69	13.54	12.03	35	2.75	14.37	14.97
7	0.82	8.51	10.92	22	1.48	7.34	4.70	36	8.02	25.84	17.52
8	1.34	12.06	22.69	23	2.08	14.00	22.81	37	8.68	15.53	13.93
9	0.51	7.84	9.59	24	1.76	9.12	14.07	38	17.23	30.02	19.07
10	1.04	6.23	6.96	25	1.42	15.17	14.71	39	3.85	12.73	11.00
11	1.30	14.27	16.91	26	9.33	33.73	36.16	40	4.79	10.96	12.83
12	1.63	6.83	6.90	27	4.91	16.34	22.91	41	8.12	16.65	18.87
13	2.45	4.14	3.68	28	4.91	20.52	24.58	42	10.74	21.77	19.35
14	9.37	25.68	32.84	29	5.67	17.37	21.82	43	3.04	16.70	11.98
15	6.78	18.26	17.36								

Table S3. Imbibed water mass and corresponding T_2 intensity changes over time during spontaneous imbibition.

No.	Time (min)	M_r	M_w	P_w	M_w/M_r	T_2 intensity	I_w-T_2	I_w-T_2/M_r	P_w-T_2
27	0	18.41	0.00	0.00	0.00	852.68	0.00	0.00	0.00
	10	18.43	0.02	8.55	0.13	941.11	88.44	4.80	7.69
	30	18.45	0.04	15.50	0.24	970.80	118.12	6.42	10.27
	60	18.47	0.06	20.49	0.31	1064.04	211.36	11.48	18.37
	120	18.49	0.08	27.69	0.42	1244.27	391.59	21.27	34.04
	240	18.52	0.11	37.99	0.58	1374.22	521.55	28.33	45.34
	480	18.55	0.14	48.43	0.74	1443.62	590.95	32.10	51.37
	720	18.57	0.16	57.27	0.87	1565.83	713.15	38.74	62.00
	1440	18.60	0.19	67.03	1.02	1702.40	849.72	46.15	73.87
	2880	18.64	0.23	80.65	1.23	1852.68	1000.00	54.32	86.93
	5760	18.66	0.25	89.99	1.37	1916.45	1063.77	57.78	92.48
	10080	18.69	0.28	100.00	1.52	2002.99	1150.32	62.48	100.00
28	0	16.99	0.00	0.00	0.00	1298.70	0.00	0.00	0.00
	10	17.03	0.04	14.59	0.26	1577.31	278.61	16.40	22.32
	30	17.06	0.07	23.59	0.42	1674.23	375.53	22.10	30.09
	60	17.09	0.10	33.25	0.60	1744.65	445.95	26.25	35.73
	120	17.12	0.13	43.79	0.78	1947.58	648.88	38.19	51.99
	240	17.16	0.17	56.41	1.01	2095.54	796.84	46.90	63.85
	480	17.19	0.20	64.29	1.15	2201.07	902.37	53.11	72.30
	720	17.21	0.22	73.59	1.32	2238.50	939.80	55.32	75.30
	1440	17.24	0.25	83.51	1.50	2322.09	1023.39	60.24	82.00
	2880	17.26	0.27	87.29	1.56	2334.94	1036.25	60.99	83.03
	5760	17.28	0.29	95.63	1.71	2449.75	1151.05	67.75	92.23
	10080	17.29	0.30	100.00	1.79	2546.76	1248.06	73.46	100.00
31	0	5.48	0.00	0.00	0.00	415.39	0.00	0.00	0.00
	10	5.49	0.02	13.40	0.28	424.07	8.68	1.58	1.88
	30	5.50	0.02	19.43	0.40	500.84	85.45	15.60	18.53
	60	5.51	0.03	27.15	0.56	542.86	127.47	23.27	27.64
31	120	5.52	0.04	39.57	0.81	614.88	199.48	36.41	43.26
	240	5.54	0.06	51.91	1.07	668.81	253.42	46.25	54.95
	480	5.55	0.07	61.49	1.26	708.00	292.61	53.40	63.45
	720	5.56	0.08	67.52	1.39	728.68	313.28	57.18	67.94
	1440	5.56	0.08	72.23	1.49	743.81	328.42	59.94	71.22
	2880	5.57	0.09	76.66	1.58	757.28	341.89	62.40	74.14
	5760	5.57	0.09	81.01	1.67	799.25	383.86	70.06	83.24
	10080	5.59	0.11	100.00	2.06	876.54	461.15	84.17	100.00
34	0	10.37	0.00	0.00	0.00	700.22	0.00	0.00	0.00
34	10	10.38	0.01	11.45	0.13	729.25	29.03	2.80	5.67
	30	10.39	0.02	18.47	0.21	771.37	71.15	6.86	13.90
	60	10.40	0.03	27.32	0.30	827.69	127.48	12.30	24.91
	120	10.41	0.05	39.46	0.44	907.43	207.22	19.99	40.49
	240	10.43	0.06	52.56	0.58	934.02	233.80	22.55	45.68
	480	10.43	0.07	59.58	0.66	1025.90	325.69	31.42	63.64
	720	10.45	0.08	70.08	0.78	1079.96	379.75	36.63	74.20
	1440	10.45	0.09	74.24	0.83	1096.68	396.47	38.25	77.46
	2880	10.46	0.10	84.74	0.94	1129.02	428.81	41.37	83.78
	5760	10.47	0.11	92.37	1.03	1154.42	454.20	43.82	88.74
	10080	10.48	0.12	100.00	1.11	1212.02	511.81	49.37	100.00

Note: M_r represents the mass of the samples. M_w denotes the mass of water imbibed at each time. P_w signifies the cumulative percentage of the imbibed water. I_w-T_2 refers to the accumulated quantity of T_2 signal corresponding to the imbibed water. P_w-T_2 indicates the cumulative percentage of the T_2 signal for the water that has penetrate the shales.

Table S4. Fitting equations, coefficients of determination (R^2), and corresponding data ranges for the two stages of spontaneous imbibition.

No.	Stage 1			Stage 2		
	Fitting equation	R^2	Time range (min)	Fitting equation	R^2	Time range (min)
27	Y=0.1153ln X-0.1451	0.9855	10-120	Y=0.2534ln X-0.8110	0.9983	240-10080
28	Y=0.2785ln X-0.5358	0.9961	30-720	Y=0.1585ln X+0.3288	0.9796	1440-10080
31	Y=0.3231ln X-0.7258	0.9945	30-480	Y=0.1332ln X+0.5143	0.9997	720-5760
34	Y=0.1787ln X-0.4130	0.9929	30-720	Y=0.1299ln X-0.0936	0.9860	1440-10080