

Supplementary Material

Supplementary Table

Table S1: Yields and carbon and hydrogen isotopic ratios of gas products during non-isothermal pyrolysis of YM201 oil with and without water in gold-tube system at a constant pressure of 50 MPa.

NO.	T (°C)	Easy%R _o ^a (%)	Gas yields (mmol/g oil)								$\delta^{13}\text{C}$ (VPDB, ‰)					$\delta^2\text{H}_1$ (VSMOW, ‰)		
			CH ₄	C ₂ H ₆	C ₃ H ₈	<i>i</i> -C ₄	<i>n</i> -C ₄	<i>i</i> -C ₅	<i>n</i> -C ₅	Alkenes ^b	H ₂	CO ₂	H ₂ S	C ₁	C ₂		C ₃	CO ₂
Series 1: Non-isothermal anhydrous pyrolysis of YM201 oil at 2 °C/h																		
1-1#	330	0.69	0.016	0.0251	0.011	0.0006	0.0018	0.0004	0.0005	0.0010	n.d.	0.028	n.d.	-50.4	-40.9	-40.1	-23.4	-319.5
1-2#	350	0.8	0.030	0.0166	0.011	0.0015	0.0043	0.0018	0.0030	0.0020	0.006	0.035	0.019	-50.9	-43.5	-40.6	-24.6	-310.1
1-3#	380	1.04	0.133	0.0726	0.072	0.0146	0.0354	0.0118	0.0169	0.0042	0.007	0.041	0.056	-51.4	-44.1	-41.2	-24.5	-300.4
1-4#	390	1.15	0.231	0.1145	0.136	0.0229	0.0520	0.0400	0.0561	0.0050	0.012	0.044	0.055	-51.6	-44.7	-41.2	-25.5	-286.9
1-5#	420	1.52	0.964	0.7830	0.842	0.1467	0.3370	0.1003	0.1154	0.0106	0.031	0.046	0.091	-51.0	-43.7	-40.7	-26.1	-264.5
1-6#	440	1.82	2.455	1.5291	1.769	0.3075	0.6125	0.1265	0.1480	0.0134	0.060	0.051	0.204	-50.3	-42.2	-38.4	-26.3	-251.9
1-7#	460	2.16	4.376	2.6255	2.105	0.4331	0.7265	0.0928	0.0883	0.0156	0.065	0.052	0.183	-49.0	-39.6	-33.9	-24.9	-233.5
1-8#	470	2.34	6.401	3.5607	2.527	0.4963	0.6994	0.0830	0.0707	0.0182	0.078	0.062	0.210	-48.4	-38.8	-32.8	-23.5	-219.6
1-9#	500	2.92	13.123	4.7818	1.976	0.0832	0.0892	0.0166	0.0150	0.0141	0.126	0.063	0.246	-46.2	-33.5	-23.3	-23.1	-176.9
1-10#	520	3.31	17.547	4.0426	0.809	0.0386	0.0409	0.0058	0.0070	0.0064	0.146	0.065	0.225	-44.0	-28.3	-14.2	-22.1	-150.4
1-11#	580	4.24	26.234	0.9596	0.013	0.0002	0.0002	0.0001	0.0001	0.0003	0.320	0.106	0.206	-38.4	-13.2	n.d.	-21.8	-113.0
1-12#	600	4.45	27.701	0.3421	0.005	0.0002	0.0002	n.d.	n.d.	0.0001	0.353	0.122	0.238	-37.1	-12.7	n.d.	-22	-102.9
1-13#	650	4.68	27.843	0.1521	0.002	0.0001	0.0001	n.d.	n.d.	n.d.	0.612	0.148	0.354	-36.3	n.d.	n.d.	n.d.	-95.2

Series 2: Non-isothermal anhydrous pyrolysis of YM201 oil at 20 °C/h

2-1#	330	0.54	0.001	0.0003	0.0002	0.0001	0.0001	0.0002	0.0004	n.d.	n.d.	0.014	n.d.	-49.1	n.d.	-39.4	-23.1	n.d.
2-2#	350	0.63	0.004	0.0014	0.0010	0.0001	0.0004	0.0002	0.0003	0.0001	n.d.	0.024	0.003	-49.5	-41.2	-40	-23.8	-320.6
2-3#	380	0.77	0.013	0.0077	0.0082	0.0015	0.0040	0.0013	0.0023	0.0015	0.002	0.032	0.007	-50.5	-42.4	-40.7	-24.9	-311.1
2-4#	400	0.89	0.053	0.0292	0.0291	0.0059	0.0142	0.0048	0.0068	0.0027	0.003	0.040	0.022	-51.0	-43.5	-41.2	-24.6	-299.9
2-5#	430	1.17	0.227	0.1357	0.1384	0.0291	0.0730	0.0256	0.0318	0.0049	0.003	0.045	0.053	-50.8	-44	-40.9	-25.5	-285.7
2-6#	450	1.4	0.733	0.5764	0.6285	0.1348	0.3118	0.0848	0.1010	0.0096	0.016	0.045	0.110	-50.9	-43.9	-40.6	-26.4	-273.1
2-7#	470	1.66	1.314	0.9564	0.9463	0.2176	0.4561	0.1104	0.1367	0.0118	0.023	0.049	0.128	-50.2	-43.7	-40.2	-26.4	-255.7
2-8#	490	1.96	3.124	2.0382	1.9965	0.3871	0.6654	0.1240	0.1634	0.0151	0.058	0.054	0.171	-49.6	-41.3	-37.9	-26.1	-235.0
2-9#	530	2.65	9.566	4.8334	1.8256	0.3136	0.3723	0.0414	0.0313	0.0155	0.110	0.055	0.229	-47.1	-36.3	-29.8	-23.4	-201.9
2-10#	560	3.21	16.325	4.6088	0.9855	0.0596	0.0626	0.0087	0.0100	0.0080	0.147	0.057	0.228	-44.6	-29.4	-17.6	-22.1	-162.1
2-11#	580	3.57	20.218	3.0860	0.1151	0.0081	0.0084	0.0005	0.0009	0.0013	0.216	0.064	0.224	-42.9	-22.1	-10.7	-21.7	-138.5
2-12#	600	3.88	24.123	2.0322	0.0349	0.0021	0.0021	0.0001	0.0002	0.0009	0.458	0.069	0.000	-40.2	-19.2	n.d.	-21.8	-121.1
2-13#	620	4.14	25.891	1.0379	0.0171	0.0008	0.0008	n.d.	n.d.	0.0002	0.361	0.090	0.223	-38.5	-13.8	n.d.	-21.9	-107.9
2-14#	650	4.45	27.487	0.3322	0.0047	0.0001	0.0001	n.d.	n.d.	n.d.	0.461	0.134	0.306	-37.0	n.d.	n.d.	-22	-100.2

Series 3: Non-isothermal pyrolysis of YM201 oil with sea water at 2 °C/h

3-1#	350	0.8	0.022	0.0202	0.0071	0.0019	0.0058	0.0014	0.0019	0.0032	0.004	0.053	0.021	-50.5	n.d.	-39.5	-27.8	-271.9
3-2#	380	1.04	0.248	0.1325	0.1232	0.0254	0.0623	0.0148	0.0190	0.0132	0.023	0.037	0.025	-50.8	-43.4	-40.6	-28.6	-282.5
3-3#	400	1.26	0.395	0.3170	0.3192	0.0563	0.1336	0.0409	0.0449	0.0205	0.032	0.081	0.155	-50.6	-43.4	-40.4	-30.5	-272.0
3-4#	420	1.52	1.096	0.7966	0.7495	0.1191	0.2946	0.1067	0.1309	0.0250	0.053	0.128	0.181	-50.1	-43.8	-40.5	-30.8	-252.4
3-5#	450	1.98	3.704	2.4017	2.1127	0.4127	0.8601	0.1677	0.1518	0.0317	0.113	0.298	0.242	-49.3	-41.9	-37.7	-30.8	-229.0
3-6#	460	2.16	5.400	3.2442	2.5318	0.4949	0.7666	0.0782	0.0727	0.0288	0.115	0.309	0.208	-48.7	-39.7	-34.1	-30	-220.1
3-7#	470	2.34	7.252	4.0739	2.8474	0.5243	0.6596	0.0563	0.0442	0.0251	0.160	0.471	0.320	-48.0	-39	-32.7	-30.8	-210.4
3-8#	500	2.92	13.535	5.0927	2.1427	0.2950	0.2890	0.0154	0.0133	0.0175	0.221	0.530	0.322	-46.1	-34.4	-24.3	-29.4	-185.3
3-9#	520	3.31	18.853	4.2575	1.0200	0.0865	0.0915	0.0076	0.0087	0.0133	0.247	0.648	0.309	-44.1	-29	-15.3	-29.5	-163.0
3-10#	580	4.24	27.883	1.5195	0.0193	0.0009	0.0009	0.0001	0.0001	0.0005	0.481	0.914	0.298	-38.3	-13.5	n.d.	-28.6	-113.6

3-11#	600	4.45	28.733	0.6367	0.0075	0.0008	0.0007	0.0002	0.0001	0.0002	0.755	1.626	0.401	-36.8	-10.8	n.d.	-28.9	-102.9
3-12#	650	4.68	29.140	0.1678	0.0015	0.0001	0.0001	n.d.	n.d.	n.d.	0.993	2.023	0.451	-36.0	n.d.	n.d.	-32.6	-91.9
Series 4: Non-isothermal pyrolysis of YM201 oil with sea water at 20 °C/h																		
4-1#	330	0.54	0.002	0.0002	0.0001	0.0001	0.0001	0.0001	0.0001	0.0002	n.d.	n.d.	n.d.	-49.4	-39.7	-37.7	-25.3	n.d.
4-2#	350	0.63	0.003	0.0013	0.0010	0.0001	0.0004	0.0001	0.0002	0.0007	0.001	0.011	0.003	-49.8	-41.1	-39.8	-26.9	-272.1
4-3#	380	0.77	0.013	0.0039	0.0024	0.0003	0.0009	0.0002	0.0004	0.0012	0.003	0.012	0.006	-50.9	-42.5	-40.3	-28.1	-283.4
4-4#	400	0.89	0.055	0.0239	0.0212	0.0038	0.0095	0.0029	0.0041	0.0082	0.008	0.023	0.024	-51.2	-42.8	-40.8	-28.7	-280.7
4-5#	420	1.07	0.280	0.1531	0.1537	0.0309	0.0654	0.0193	0.0202	0.0160	0.028	0.043	0.026	-50.9	-43.9	-41.4	-28.7	-278.9
4-6#	440	1.28	0.446	0.3631	0.3658	0.0649	0.1477	0.0377	0.0410	0.0210	0.036	0.092	0.173	-50.6	-43.6	-40.4	-30.6	-269.1
4-7#	460	1.53	1.115	0.8244	0.7556	0.1275	0.3024	0.1069	0.1308	0.0250	0.053	0.165	0.239	-50.6	-44	-40.2	-30.6	-259.5
4-8#	470	1.66	1.965	1.2775	1.3756	0.2239	0.5558	0.1498	0.1459	0.0292	0.060	0.175	0.162	-50.4	-43.2	-39	-31.1	-247.7
4-9#	500	2.13	5.139	3.0348	2.5057	0.5112	0.9416	0.0805	0.0723	0.0299	0.124	0.220	0.216	-48.9	-39.7	-34.1	-31.3	-221.5
4-10#	520	2.47	8.810	4.6854	2.9040	0.4915	0.5819	0.0297	0.0213	0.0220	0.187	0.396	0.226	-47.8	-37.3	-31	-30.6	-211.2
4-11#	580	3.57	21.852	3.6884	0.1687	0.0061	0.0106	0.0006	0.0011	0.0041	0.290	0.580	0.236	-42.2	-23.7	-10.2	-29	-146.8
4-12#	600	3.88	24.886	2.5884	0.0473	0.0015	0.0035	0.0002	0.0004	0.0016	0.489	0.740	0.267	-40.1	-20.3	n.d.	-28.2	-125.5
4-13#	650	4.45	28.672	0.5429	0.0052	0.0001	0.0002	0.0001	n.d.	n.d.	0.828	1.169	0.365	-37.1	-13.8	n.d.	-30.3	-99.4
Series 5: Non-isothermal pyrolysis of YM201 oil with deionized water at 20 °C/h																		
5-1#	330	0.54	0.001	0.0003	0.0002	0.0001	0.0001	0.0001	0.0002	0.0003	0.000	0.017	0.000	n.d.	n.d.	n.d.	-25.5	n.d.
5-2#	350	0.63	0.005	0.0009	0.0008	0.0001	0.0004	0.0001	0.0002	0.0007	0.001	0.027	0.003	-49.7	-40.8	-39.8	-26.8	n.d.
5-3#	380	0.77	0.047	0.0067	0.0053	0.0008	0.0022	0.0006	0.0012	0.0029	0.003	0.028	0.010	-50.5	-42.5	-40.9	-28.3	n.d.
5-4#	400	0.89	0.115	0.0356	0.0369	0.0075	0.0186	0.0061	0.0090	0.0102	0.008	0.047	0.036	-51.0	-43.5	-41	-28.7	n.d.
5-5#	420	1.07	0.389	0.1877	0.2224	0.0508	0.1275	0.0445	0.0560	0.0160	0.011	0.070	0.086	-50.8	-43.8	-40.6	-29.3	n.d.
5-6#	450	1.4	1.142	0.6615	0.6502	0.1181	0.2930	0.0983	0.1219	0.0257	0.075	0.143	0.250	-50.6	-43.9	-40.2	-30.2	-267.1
5-7#	470	1.66	2.043	1.2968	1.4143	0.2419	0.5773	0.1637	0.2223	0.0274	0.061	0.202	0.158	-50.3	-42.7	-38.7	-30.3	-256.1
5-8#	480	1.81	3.091	2.0765	2.0212	0.3428	0.8115	0.1236	0.1619	0.0303	0.091	0.236	0.173	-49.9	-42.7	-38.2	-31	-248.5
5-9#	550	3.03	16.461	4.5748	1.8520	0.2079	0.4642	0.0070	0.0086	0.0148	0.216	0.512	0.247	-45.0	-30.7	-20.2	-29.4	-187.6

5-10#	580	3.57	21.454	3.6279	0.0868	0.0029	0.0068	0.0006	0.0014	0.0050	0.357	0.619	0.259	-42.7	-24.1	-12.4	-28.7	-161.7
5-11#	600	3.88	24.735	2.9485	0.0306	0.0006	0.0024	0.0002	0.0006	0.0022	0.812	0.737	0.257	-41.1	-20.4	n.d.	-28.7	-148.6
5-12#	620	4.14	27.300	1.3643	0.0144	0.0002	0.0007	0.0001	0.0002	0.0004	0.591	0.790	0.270	-38.5	-15	n.d.	-29	-125.4
5-13#	650	4.45	28.607	0.4325	0.0042	0.0001	0.0001	n.d.	n.d.	n.d.	0.777	1.437	0.309	-37.0	-14.5	n.d.	-30.3	-110.1

^a The equivalent vitrinite reflectance values (Eas_y%R_o) for each heated sample was calculated according to the kinetic parameters from Sweeney and Burnham (1990) and the respective temperature/time conditions. The amounts of *oil* and water loaded in pyrolysis were 30 mg and 10 mg, respectively. ^b Alkenes refer to alkene gases including ethylene (C₂H₄), propylene (C₃H₆), butylenes (C₄H₈), methylbutenes and pentenes (C₅H₁₀). n.d. means lower than 0.0001 mmol/g oil for gas yields and no detectable data for isotopic ratios.