

Supplementary Materials (SM)
for
**Degradation of Tetrabromobisphenol A (TBBA) with Calcium
Hydroxide: A Thermo-kinetic Analysis**

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Supplementary materials

Table S1 Kinetic parameters of TBBA and TBBA:Ca(OH)₂ via KAS, FWO and Starink method in pyrolysis process

TBBA									
α	KAS Model			FWO Model			Starink model		
	R^2	E_a	A	R^2	E_a	A	R^2	E_a	A
		kJ/mol	min⁻¹		kJ/mol	min⁻¹		kJ/mol	min⁻¹
0.05	0.99	124.06	1.61E+12	0.99	133.38	1.18E+13	0.99	1241.44	1.74E+12
0.1	0.99	120.14	6.94E+11	0.99	129.56	5.23E+12	0.99	120.52	7.53E+11
0.15	0.99	117.72	4.13E+11	0.99	127.21	3.16E+12	0.99	118.09	4.47E+11
0.2	0.99	117.21	3.70E+11	0.99	126.76	2.87E+12	0.99	117.59	4.02E+11
0.25	0.99	116.51	3.19E+11	0.99	126.09	2.49E+12	0.99	116.89	3.46E+11
0.3	0.99	116.42	3.13E+11	0.99	126.03	2.45E+12	0.99	116.81	3.39E+11
0.35	0.99	116.01	2.86E+11	0.99	125.64	2.26E+12	0.99	116.39	3.1E+11
0.4	0.99	115.46	2.54E+11	0.99	125.12	2.02E+12	0.99	115.84	2.76E+11
0.45	0.99	115.37	2.5E+11	0.99	125.05	1.99E+12	0.99	115.76	2.71E+11
0.5	0.99	115.56	2.6E+11	0.99	125.27	2.08E+12	0.99	115.95	2.82E+11
0.55	0.99	117.22	3.71E+11	0.99	126.95	2.99E+12	0.99	117.61	4.03E+11
0.6	0.99	113.29	1.61E+11	0.99	123.13	1.32E+12	0.99	113.69	1.74E+11
0.65	0.87	77.61	6.98E+07	0.9	88.15	6.95E+08	0.87	78.04	7.65E+07
0.7	0.9	100.96	1.12E+10	0.92	112.81	1.44E+11	0.9	101.43	1.24E+10
0.75	0.92	140.23	5.10E+13	0.92	153.18	8.04E+14	0.92	140.75	5.70E+13
0.8	0.21	62.76	2.63E+06	0.29	77.54	6.86E+06	0.20	63.35	3.01E+06

TBBA:Ca(OH)₂

α	KAS Model			FWO Model			Starink model		
	R^2	Ea	A	R^2	Ea	A	R^2	Ea	A
		kJ/mol	min⁻¹		kJ/mol	min⁻¹		kJ/mol	min⁻¹
0.05	0.95	85.68	2.56E+08	0.96	95.23	1.94E+09	0.95	86.07	2.77E+08
0.1	0.97	84.85	2.14E+08	0.98	94.66	1.72E+09	0.97	85.24	2.33E+08
0.15	0.98	32.21	2.02E+03	0.98	42.62	2.18E+04	0.97	32.62	2.23E+03
0.2	0.72	16.09	3.94E+01	0.89	29.18	9.99E+02	0.73	16.61	4.52E+01
0.25	0.92	60.63	1.16E+06	0.94	75.24	2.73E+07	0.92	61.21	1.32E+02
0.3	0.91	91.73	9.24E+08	0.93	107.11	2.38E+10	0.91	92.34	1.05E+09

Table S2 Kinetic parameters of TBBA and TBBA:Ca(OH)₂ via KAS, FWO, and Starink method in Combustion process

TBBA									
α	KAS Model			FWO Model			Starink model		
	R^2	Ea	A	R^2	Ea	A	R^2	Ea	A
		kJ/mol	min⁻¹		kJ/mol	min⁻¹		kJ/mol	min⁻¹
0.05	0.81	188.08	1.26E+18	0.82	197.39	9.04E+18	0.81	188.45	1.37E+18
0.1	0.77	180.14	2.36E+17	0.78	189.62	1.74E+18	0.77	180.51	2.56E+17
0.15	0.76	169.46	2.46E+16	0.77	179.01	1.86E+17	0.76	169.85	2.67E+16
0.2	0.76	163.06	6.34E+15	0.78	172.67	4.85E+16	0.76	163.45	6.88E+15
0.25	0.77	157.72	2.03E+15	0.79	167.34	1.57E+16	0.77	158.09	2.21E+15
0.3	0.77	153.98	9.23E+14	0.79	163.65	7.19E+15	0.77	154.37	1E+15
0.35	0.78	151.04	4.94E+14	0.8	160.74	3.88E+15	0.78	151.42	5.36E+14
0.4	0.78	147.83	2.5E+14	0.8	157.56	1.97E+15	0.78	148.22	2.71E+14
0.45	0.78	146.12	1.73E+14	0.8	155.87	1.38E+15	0.78	146.51	1.88E+14
0.5	0.78	144.16	1.14E+14	0.8	153.93	9.13E+14	0.78	144.55	1.24E+14
0.55	0.78	142.42	7.88E+13	0.8	152.23	6.36E+14	0.78	142.81	8.57E+13

0.6	0.83	127.73	3.43E+12	0.85	137.71	2.89E+13	0.83	128.13	3.74E+12
0.65	0.87	125.17	1.98E+12	0.89	136.06	2.03E+13	0.87	125.59	2.18E+12
0.7	0.86	119.18	5.5E+11	0.89	130.82	6.62E+12	0.87	119.65	6.08E+11
0.75	0.83	105.17	2.71E+10	0.87	117.34	3.71E+11	0.84	105.65	3.01E+10
0.8	0.82	98.59	6.56E+09	0.86	111.17	9.87E+10	0.82	99.11	7.32E+09
0.85	0.82	99.42	7.84E+09	0.86	112.28	1.25E+11	0.83	99.93	8.74E+09
0.9	0.83	101.69	1.28E+10	0.86	114.81	2.15E+11	0.83	102.21	1.43E+10
0.95	0.82	99.99	8.87E+09	0.86	113.41	1.6E+11	0.82	100.53	9.97E+09

TBBA:Ca(OH)₂

α	KAS Model			FWO Model			Starink model		
	R^2	Ea	A	R^2	Ea	A	R^2	Ea	A
		kJ/mol	min⁻¹		kJ/mol	min⁻¹		kJ/mol	min⁻¹
0.05	0.98	88.89	5.02E+08	0.99	98.45	3.80E+09	0.98	89.28	5.45E+08
0.1	0.98	97.39	3.04E+09	0.98	107.21	2.41E+10	0.98	97.79	3.30E+09
0.15	0.97	57.59	5.98E+05	0.98	67.79	5.49E+06	0.97	58.01	6.54E+05
0.2	0.3	9.01	5.30E+6	0.72	21.46	1.55E+02	0.32	9.50	6.18E+06
0.25	0.8	13.58	2.01E+01	0.92	26.80	5.68E+02	0.8	14.35	2.4E+01
0.3	0.99	55.27	3.59E+05	0.99	69.92	8.69E+06	0.99	55.86	4.09E+05
0.35	0.99	65.87	3.61E+06	0.99	80.94	9.23E+07	0.99	66.47	4.12E+06
0.4	0.99	73.52	1.87E+07	0.99	88.89	5.02E+08	0.99	74.12	2.13E+07
0.45	0.99	76.98	3.95E+07	0.99	92.64	1.11E+09	0.99	77.61	4.52E+07
0.5	0.99	75.43	2.83E+07	0.99	91.36	8.48E+08	0.99	76.07	3.25E+07
0.55	0.99	71.66	1.26E+07	0.99	87.87	4.04E+08	0.99	72.31	1.45E+07
0.6	0.99	68.38	6.22E+06	0.99	84.87	2.14E+08	0.99	69.04	7.18 E+06

Table S3 Thermodynamics parameters of TBBA and TBBA:Ca(OH)₂ via KAS, FWO, and Starink method in pyrolysis process

TBBA									
KAS Model			FWO Model				Starink model		
α	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
0.05	119.3005	133.8686	-0.02497	128.6205	133.5173	-0.00839	119.6746	133.854	-0.02431
0.1	115.3763	134.0245	-0.03197	124.8044	133.6581	-0.01518	115.7587	134.0091	-0.03128
0.15	112.9569	134.1232	-0.03628	122.4515	133.747	-0.01936	113.331	134.1078	-0.03562
0.2	112.4498	134.1441	-0.03719	121.9942	133.7644	-0.02018	112.8322	134.1283	-0.03651
0.25	111.7514	134.1731	-0.03844	121.3374	133.7896	-0.02135	112.1338	134.1572	-0.03775
0.3	111.6599	134.1769	-0.0386	121.2709	133.7922	-0.02146	112.0424	134.161	-0.03792
0.35	111.2442	134.1942	-0.03934	120.8802	133.8072	-0.02216	111.6267	134.1783	-0.03866
0.4	110.6955	134.2172	-0.04032	120.3564	133.8275	-0.02309	111.0779	134.2012	-0.03964
0.45	110.6124	134.2207	-0.04047	120.2899	133.8301	-0.02321	110.9948	134.2047	-0.03979
0.5	110.8036	134.2127	-0.04013	120.506	133.8217	-0.02283	111.186	134.1967	-0.03944
0.55	112.4581	134.1438	-0.03717	122.1938	133.7568	-0.01982	112.8488	134.1276	-0.03648
0.6	108.5339	134.3089	-0.04418	118.3693	133.9051	-0.02663	108.9329	134.2919	-0.04347
0.65	72.85267	136.1434	-0.10849	83.38402	135.5263	-0.08938	73.27419	136.1172	-0.10773
0.7	96.19589	134.8681	-0.06629	108.0433	134.3299	-0.04506	96.66979	134.8454	-0.06544
0.75	135.4712	133.2744	0.003766	148.4161	132.8461	0.02669	135.9867	133.2566	0.00468
0.8	57.99805	137.1738	-0.13572	72.77868	136.1481	-0.10863	58.58917	137.1283	-0.13463
TBBA:Ca(OH) ₂									
KAS Model			FWO Model				Starink model		
α	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
0.05	79.59283	139.3033	-0.09994	89.1373	138.7786	-0.08308	79.97528	139.2811	-0.09926
0.1	78.76143	139.3517	-0.10141	88.57195	138.8082	-0.08408	79.15219	139.3289	-0.10072

0.15	26.1097	144.1648	-0.19759	36.52964	142.7721	-0.17782	26.52706	144.1008	-0.19678
0.2	9.996338	147.6119	-0.23033	23.09255	144.6535	-0.20346	10.52012	147.4528	-0.22918
0.25	54.53527	141.0217	-0.14475	69.14463	139.9492	-0.11851	55.11642	140.9743	-0.1437
0.3	85.63711	138.9646	-0.08925	101.0097	138.195	-0.06224	86.25235	138.9314	-0.08817

Table S4 Thermodynamics parameters of TBBA and TBBA:Ca(OH)₂ via KAS, FWO, and Starink method in combustion process

TBBA									
α	KAS Model			FWO Model			Starink model		
	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
0.05	182.3248	131.9973	0.086185	191.6365	131.7627	0.102533	182.6989	131.9876	0.086842
0.1	174.3849	132.2067	0.072229	183.8462	131.9582	0.088857	174.759	132.1966	0.072887
0.15	163.7097	132.5033	0.05344	173.2542	132.2373	0.070241	164.0922	132.4923	0.054114
0.2	157.3079	132.6902	0.042157	166.9106	132.4124	0.059078	157.6904	132.6789	0.042832
0.25	151.9454	132.8526	0.032696	161.5897	132.5644	0.049705	152.3362	132.8406	0.033386
0.3	148.2291	132.9684	0.026134	157.8982	132.6727	0.043198	148.6115	132.9563	0.026809
0.35	145.2859	133.0621	0.020933	154.9883	132.7598	0.038066	145.6683	133.0498	0.021609
0.4	142.0767	133.1663	0.015259	151.8041	132.8569	0.032447	142.4675	133.1535	0.01595
0.45	140.364	133.2229	0.012229	150.1163	132.9092	0.029467	140.7548	133.2099	0.01292
0.5	138.4102	133.2883	0.008771	148.1792	132.9699	0.026046	138.801	133.2751	0.009463
0.55	136.6643	133.3474	0.00568	146.4748	133.024	0.023034	137.055	133.3341	0.006372
0.6	121.9734	133.876	-0.02038	131.9586	133.5105	-0.00266	122.3725	133.8608	-0.01967
0.65	119.4127	133.9743	-0.02494	130.3041	133.5692	-0.00559	119.8451	133.9575	-0.02417
0.7	113.4267	134.2122	-0.03559	125.0496	133.7604	-0.01492	113.8922	134.1933	-0.03477
0.75	99.40925	134.8197	-0.06064	111.5893	134.2876	-0.03887	99.89978	134.7971	-0.05976
0.8	92.84119	135.1328	-0.07242	105.4203	134.5498	-0.04988	93.34834	135.1079	-0.07151

0.85	93.66428	135.0924	-0.07094	106.526	134.5018	-0.04791	94.17143	135.0677	-0.07003
0.9	95.934	134.9828	-0.06687	109.0535	134.3937	-0.04339	96.45778	134.9579	-0.06593
0.95	94.23794	135.0645	-0.06991	107.6567	134.4531	-0.04589	94.77835	135.0383	-0.06894

TBBA:Ca(OH)₂

α	KAS Model			FWO Model			Starink model		
	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol	kJ/mol
0.05	82.36555	139.177	-0.09505	91.91834	138.6698	-0.07822	82.74799	139.1557	-0.09437
0.1	90.86246	138.7234	-0.08008	100.673	138.2464	-0.06286	91.25322	138.7035	-0.07939
0.15	51.06667	141.3337	-0.15102	61.2721	140.5231	-0.13259	51.47488	141.2986	-0.15028
0.2	2.475494	150.5559	-0.24775	14.93485	146.239	-0.21968	2.973502	150.2884	-0.24647
0.25	7.056508	148.5119	-0.23667	20.28159	145.1336	-0.20889	7.824721	148.2386	-0.23492
0.3	48.7429	141.5384	-0.15525	63.40049	140.3695	-0.12878	49.32987	141.4859	-0.15418
0.35	59.34076	140.6667	-0.13606	74.41404	139.6427	-0.10913	59.94352	140.6214	-0.13498
0.4	66.97301	140.1219	-0.12238	82.36555	139.177	-0.09505	67.58825	140.0804	-0.12129
0.45	70.45242	139.892	-0.11618	86.11516	138.9717	-0.08843	71.0793	139.8517	-0.11506
0.5	68.90352	139.993	-0.11894	84.83481	139.0409	-0.09069	69.54037	139.9513	-0.1178
0.55	65.13395	140.2478	-0.12567	81.34293	139.2345	-0.09686	65.78245	140.203	-0.12451
0.6	61.85574	140.4805	-0.13155	78.34989	139.4067	-0.10215	62.51588	140.4327	-0.13036

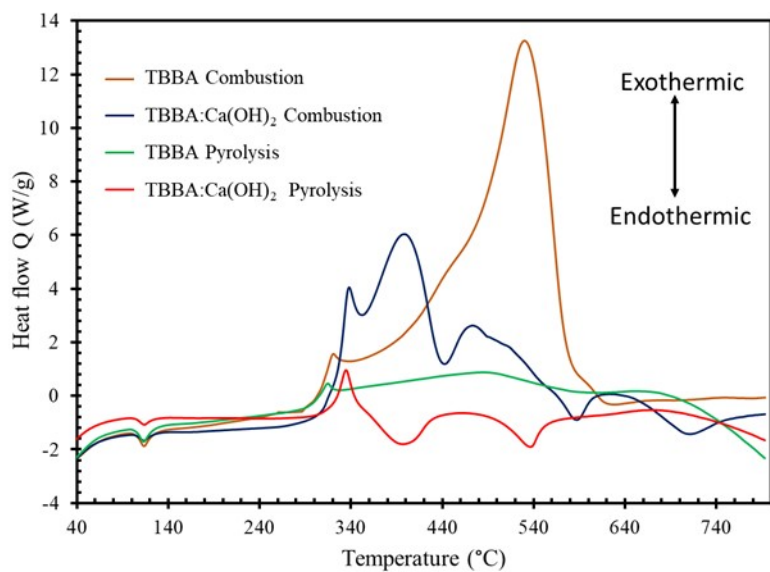


Fig. S1 DSC curve for the four samples during pyrolysis and combustion

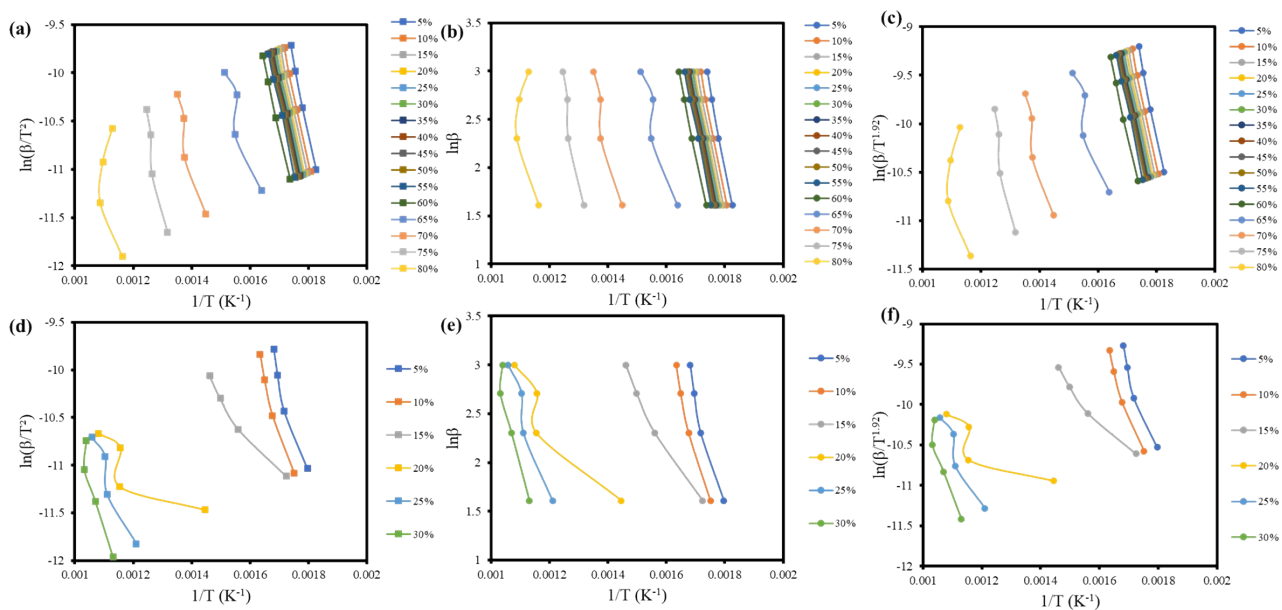


Fig. S2 Isoconversional curves for pyrolysis of TBBA (a) KAS, (b) FWO and (c) Starink, and for pyrolysis of TBBA:Ca(OH)₂ (d) KAS, (e) FWO and (f) Starink models

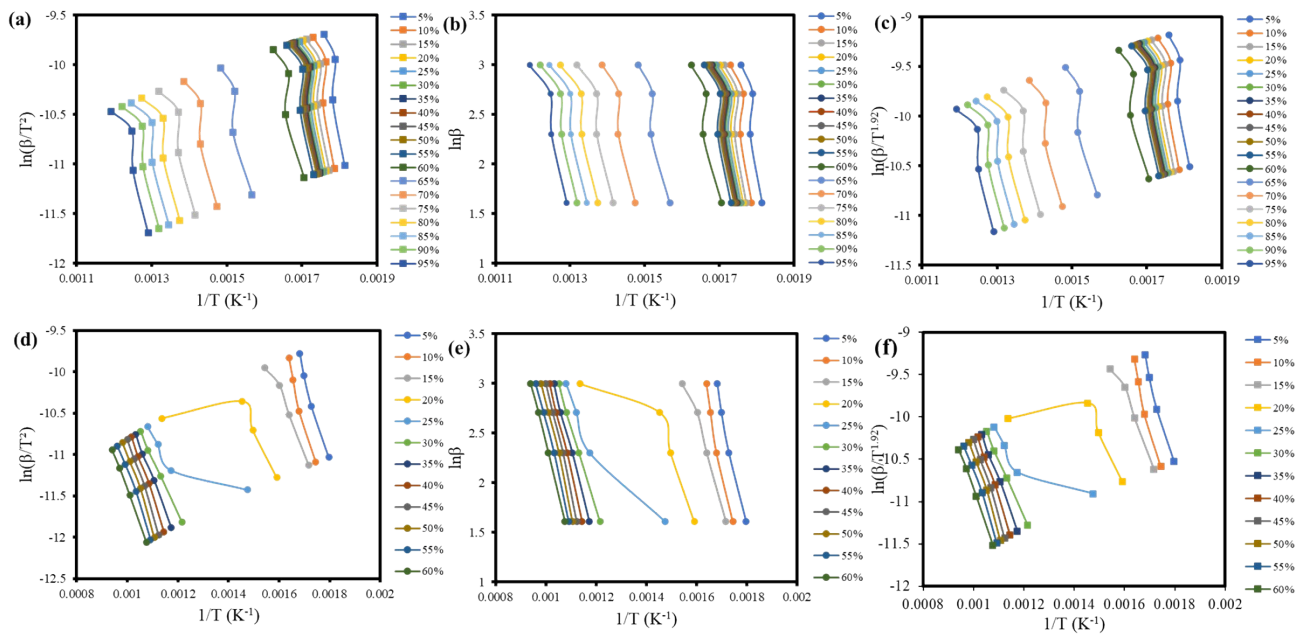


Fig. S3 Isoconversional curves for combustion of TBBA (a) KAS, (b) FWO and (c) Starink, and for combustion of TBBA:Ca(OH)₂ (d) KAS, (e) FWO and (f) Starink models