

Supporting information

Desorption Kinetics of Naphthalene and Acenaphthene over Two Activated Carbons via thermogravimetric analysis

Ziyi Li,[†] Yingshu Liu,[†] Xiong Yang,^{*,†} Yi Xing,[‡] Zhanying Wang,[†] Quan Yang,[†] Ralph T. Yang,[§]

[†]School of Mechanical Engineering, and [‡]School of Civil and Environmental Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China

[§]Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan 48109-2136, United States

Corresponding Author

*Telephone: +86-10-62332730. Fax: +86-10-62334210. E-mail: yangx@ustb.edu.cn.

The model fitting results

The results of the model fitting based on Coats and Redfern method for AC_{WY} and AC_{NT} are listed in Table S1 and Table S2, respectively. Six models, D3, AE1.5, AE2, AE3, AE4 and F2, giving linear fit with squared correlation coefficient (r^2) larger than 0.98, are selected. The activation energy, $E_{a,i}$, and the pre-exponent factor, $\ln A_i$, obtained by each model at each heating rate based on the experimental desorption data also can be seen in the tables.

Table S1 Model's values of kinetic parameters and fitting correlation coefficient obtained using the Coats-Redfern method for AC_{WY}

model	Naphthalene on AC _{WY}			Acenaphthene on AC _{WY}		
	E_a (kJ/mol)	$\ln A$ (min ⁻¹)	r^2	E_a (kJ/mol)	$\ln A$ (min ⁻¹)	r^2
$\beta=8$ K/min						
D3	77.77±1.99	13.51±2.05	0.9876	96.44±1.94	11.42±2	0.9912
AE1.5	48.95±2.01	8.63±0.11	0.9951	61.15±2.11	5.89±0.08	0.997
AE2	68.22±2.65	13.11±0.04	0.9988	84.8±2.11	10.81±0.03	0.9987
AE3	106.75±3.92	21.85±0.04	0.9900	132.11±4.11	20.44±0.03	0.9928
AE4	145.27±5.19	30.44±0.02	0.9906	179.42±5.45	29.93±0.01	0.9932
F2	45.49±0.57	8.48±2.58	0.9889	56.74±0.76	5.63±2.51	0.992
$\beta=12$ K/min						
D3	78.83±1.88	13.76±2.05	0.9886	96.73±1.78	11.41±2.01	0.9922
AE1.5	49.62±1.95	8.93±0.11	0.9957	61.3±1.78	6.02±0.08	0.9975
AE2	69.16±2.56	13.38±0.04	0.9988	85.07±2.62	10.86±0.03	0.9984
AE3	108.26±3.79	22.06±0.04	0.9909	132.61±3.87	20.32±0.03	0.9937
AE4	147.35±5.02	30.6±0.02	0.9914	180.16±5.12	29.65±0.01	0.994
F2	46.06±0.58	8.77±2.61	0.9899	56.8±0.84	5.75±2.54	0.993
$\beta=16$ K/min						
D3	79.43±1.75	13.67±2.07	0.9897	98.24±1.66	11.59±2.02	0.9930
AE1.5	49.96±1.86	8.95±0.11	0.9964	62.26±1.91	6.23±0.08	0.9979
AE2	69.70±2.45	13.33±0.04	0.9988	86.42±2.51	11.05±0.03	0.9981
AE3	109.18±3.61	21.87±0.04	0.9919	134.74±3.71	20.48±0.03	0.9944
AE4	148.65±4.78	30.27±0.02	0.9923	183.07±4.91	29.77±0.01	0.9946
F2	46.32±0.6	8.8±2.65	0.9909	57.64±0.91	5.95±2.56	0.9937
$\beta=20$ K/min						
D3	79.18±1.66	13.66±2.07	0.9903	98.84±1.62	11.65±2.02	0.9933
AE1.5	49.78±1.8	9.02±0.11	0.9967	62.63±1.88	6.34±0.08	0.998
AE2	69.48±2.37	13.35±0.04	0.9988	86.95±2.47	11.13±0.03	0.998
AE3	108.89±3.49	21.79±0.04	0.9924	135.6±3.65	20.5±0.03	0.9946
AE4	148.3±4.62	30.1±0.02	0.9928	184.25±4.82	29.73±0.01	0.9949
F2	46.12±0.6	8.86±2.68	0.9914	57.94±0.95	6.07±2.58	0.9940

Table S2 Model's values of kinetic parameters and fitting correlation coefficient obtained using the Coats-Redfern method for AC_{NT}

model	Naphthalene on AC _{NT}			Acenaphthene on AC _{NT}		
	E _a (kJ/mol)	lnA (min ⁻¹)	r ²	E _a (kJ/mol)	ln A (min ⁻¹)	r ²
$\beta=8$ K/min						
D3	52.4±0.69	3.16±2.31	0.9974	89.56±0.56	9.03±2.06	0.9994
AE1.5	32.16±0.6	0.24±0.18	0.9901	56.55±1.19	4.27±0.07	0.9934
AE2	45.82±0.83	3.44±0.15	0.992	78.81±1.54	8.71±0.03	0.9943
AE3	73.14±1.06	9.62±0.05	0.9935	123.32±2.24	17.36±0.03	0.9951
AE4	100.46±1.52	15.64±0.05	0.9942	167.83±2.94	25.88±0.01	0.9954
F2	29.36±0.75	0.22±3.51	0.9903	52.06±1.03	4.02±2.72	0.9945
$\beta=12$ K/min						
D3	52.66±	3.40±	0.9997	89.28±0.43	9.15±2.06	0.9997
AE1.5	32.31±	0.51±	0.9947	56.35±1.06	4.48±0.07	0.9947
AE2	46.06±	3.70±	0.9955	78.57±1.37	8.86±0.03	0.9955
AE3	73.54±	9.83±	0.9961	123.03±1.98	17.40±0.03	0.9961
AE4	101.03±	15.81±	0.9964	167.48±2.6	25.80±0.01	0.9964
F2	29.47±	0.49±	0.9929	51.80±1.13	4.23±2.76	0.9929
$\beta=16$ K/min						
D3	52.92±0.69	3.64±2.33	0.9975	91.49±0.39	9.49±2.05	0.9997
AE1.5	32.46±0.55	0.78±0.18	0.9919	57.84±0.72	4.81±0.06	0.9977
AE2	46.29±0.76	3.95±0.14	0.9935	80.62±0.92	9.21±0.02	0.998
AE3	73.95±0.96	10.04±0.05	0.9948	126.19±1.31	17.79±0.02	0.9984
AE4	101.61±1.38	15.99±0.05	0.9953	171.75±1.7	26.23±0.01	0.9985
F2	29.58±0.86	0.76±3.58	0.9875	53.01±1.49	4.52±2.77	0.9882
$\beta=20$ K/min						
D3	53.37±0.69	3.82±2.33	0.9975	91.98±0.44	9.82±2.05	0.9997
AE1.5	32.74±0.53	0.97±0.17	0.9927	58.14±0.88	5.11±0.06	0.9966
AE2	46.69±0.73	4.14±0.14	0.9941	81.02±1.12	9.52±0.02	0.9971
AE3	74.6±0.93	10.22±0.05	0.9953	126.79±1.62	18.15±0.02	0.9976
AE4	102.5±1.32	16.15±0.05	0.9958	172.56±2.11	26.63±0.01	0.9978
F2	29.81±0.91	0.95±3.6	0.9863	53.35±1.4	4.82±2.76	0.9897