## Supporting Information

Corresponding to Environmental Science and Technology Manuscipt "Intercorrelations among Degree of Geochemical Alteration, Physicochemical Property and Organic Sorption Equilibrium of Kerogen" by Chen Yang[1], Weilin Huang[2], Baohua Xiao[2], Zhiqiang Yu[1], Ping'an Peng[1], Jiamo Fu[1], Guoying Sheng[1]

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**TABLE SI-1. Contents of Functional Groups by CP/MAS $^{13}$C-NMR.**

| Sample | Aliphatic-C | Methoxyl-C | Carbohydrate-C | Aromatic-C | Aromatic-C[a] | Carboxyl-C | Carbonyl-C | Aromaticity $f_a$[b] |
|---|---|---|---|---|---|---|---|---|
| | 0-45ppm | 45-63ppm | 63-93ppm | 93-148ppm | 148-165ppm | 165-187ppm | 187-220ppm | % |
| XFL0 | 33.1 | 7.36 | 4.75 | 25.1 | 11.7 | 8.63 | 9.34 | 44.9 |
| XFL1 | 33.7 | 7.06 | 3.51 | 25.7 | 12.5 | 8.44 | 9.15 | 46.3 |
| XFL2 | 33.4 | 7.19 | 2.58 | 26.5 | 11.8 | 6.48 | 12.1 | 47.0 |
| XFL3 | 25.5 | 5.13 | 3.36 | 29.2 | 17.4 | - | 19.3 | 57.8 |
| XFL4 | 16.7 | 3.73 | 7.26 | 44.3 | 8.65 | - | 19.4 | 65.7 |
| XFL5 | 8.16 | - | 10.7 | 50.5 | 7.77 | - | 22.9 | 75.5 |
| XFL6 | 5.51 | - | 12.1 | 58.4 | 3.84 | - | 20.2 | 77.9 |
| XFL7 | 4.99 | - | 10.6 | 62.0 | 2.28 | - | 20.1 | 80.5 |

[a]oxygen-substituted aromatic. [b] Aromaticity $f_a$ is the ratio of the peak area integrated over 93 to 165ppm as the aromatic carbon region to that over 0 to 165ppm as the total carbon region.

**TABLE SI-2. Peak Assignments for FTIR Spectra.**

| functional group | frequency range ($cm^{-1}$) | bond action |
|---|---|---|
| carboxylic | ~3400 | O-H stretching of COOH |
| aliphatic | ~2980 | C-H stretching of aliphatic |
| carboxylic | ~1700 | C=O stretching of COOH |
| aromatic | ~1600 | C=C stretching of aromatic ring |
| aliphatic | ~1400 | C-H bending of branched aliphatic |
| aromatic | 750~860 | C-H bending of aromatic ring |

**TABLE SI-3. List of Dual Mode Model Parameters of the Measured Sorption Isotherms**

| Sample | $K_{D,L}$ [a] | $Q_a$ [o b] | $b$ [c] | $R^2$ |
|---|---|---|---|---|
| | | Phenanthrene | | |
| XFL0 | 36.5 (1.42) [d] | 5499 (740) | 0.033 (0.009) | 0.998 |
| XFL1 | 38.9 (1.36) | 14544 (1195) | 0.013 (0.002) | 0.998 |
| XFL2 | 51.8 (3.79) | 14603 (1843) | 0.017 (0.005) | 0.996 |
| XFL3 | 42.2 (2.38) | 25780 (3205) | 0.014 (0.003) | 0.993 |
| XFL4 | 24.4 (2.38) | 24230 (1851) | 0.020 (0.004) | 0.993 |
| XFL5 | 6.50 (0.83) | 4242 (333) | 0.067 (0.014) | 0.987 |
| XFL6 | 3.33 (0.18) | 1231 (52) | 0.372 (0.070) | 0.989 |
| XFL7 | 2.82 (0.22) | 1400 (67) | 0.293 (0.072) | 0.977 |
| | | 1,3,5-trichlorobenznene | | |
| XFL0 | 4.24 (0.94) | 2075 (1298) | 0.0042 (0.0033) | 0.995 |
| XFL1 | 7.57 (0.62) | 2089 (650) | 0.0067 (0.0031) | 0.998 |
| XFL3 | 21.6 (1.22) | 4122 (738) | 0.0196 (0.0069) | 0.998 |
| XFL5 | 5.22 (1.60) | 6060 (1515) | 0.0083 (0.0032) | 0.990 |
| XFL7 | 1.44 (0.35) | 2472 (495) | 0.0077 (0.0030) | 0.987 |

[a] Units in (μg/g)/(μg/L) or (L/g). [b] Units in (μg/g). [c] Units in (L/μg). [d] one standard deviation

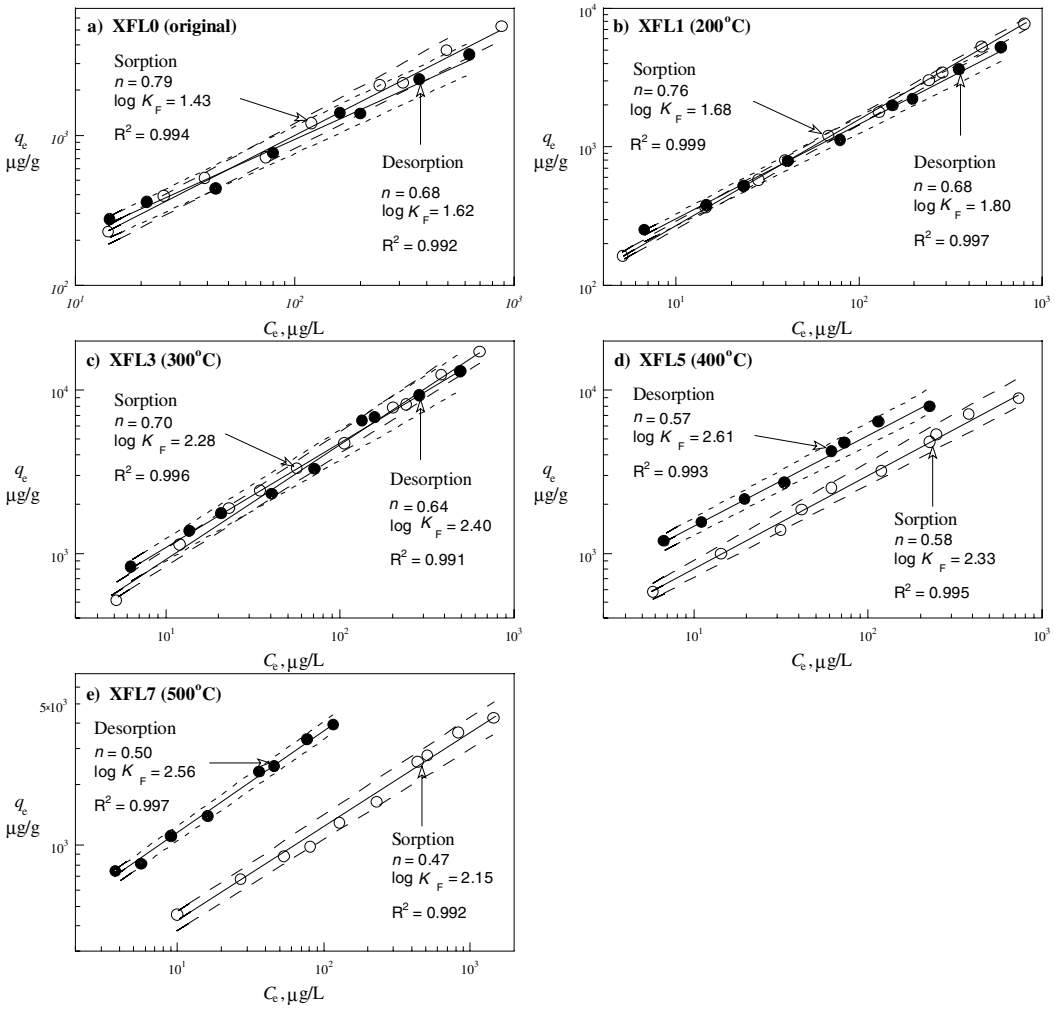


FIGURE SI-1. TCB sorption and desorption isotherms measured for five kerogen samples. The empty and filled circles represent the measured sorption and desorption data, respectively. The dashed lines are the best fits of the data sets to the Freundlich isotherm model, and the dashed lines represent the best fit isotherms ±one standard deviations of the log$K_F$ and $n$ values.

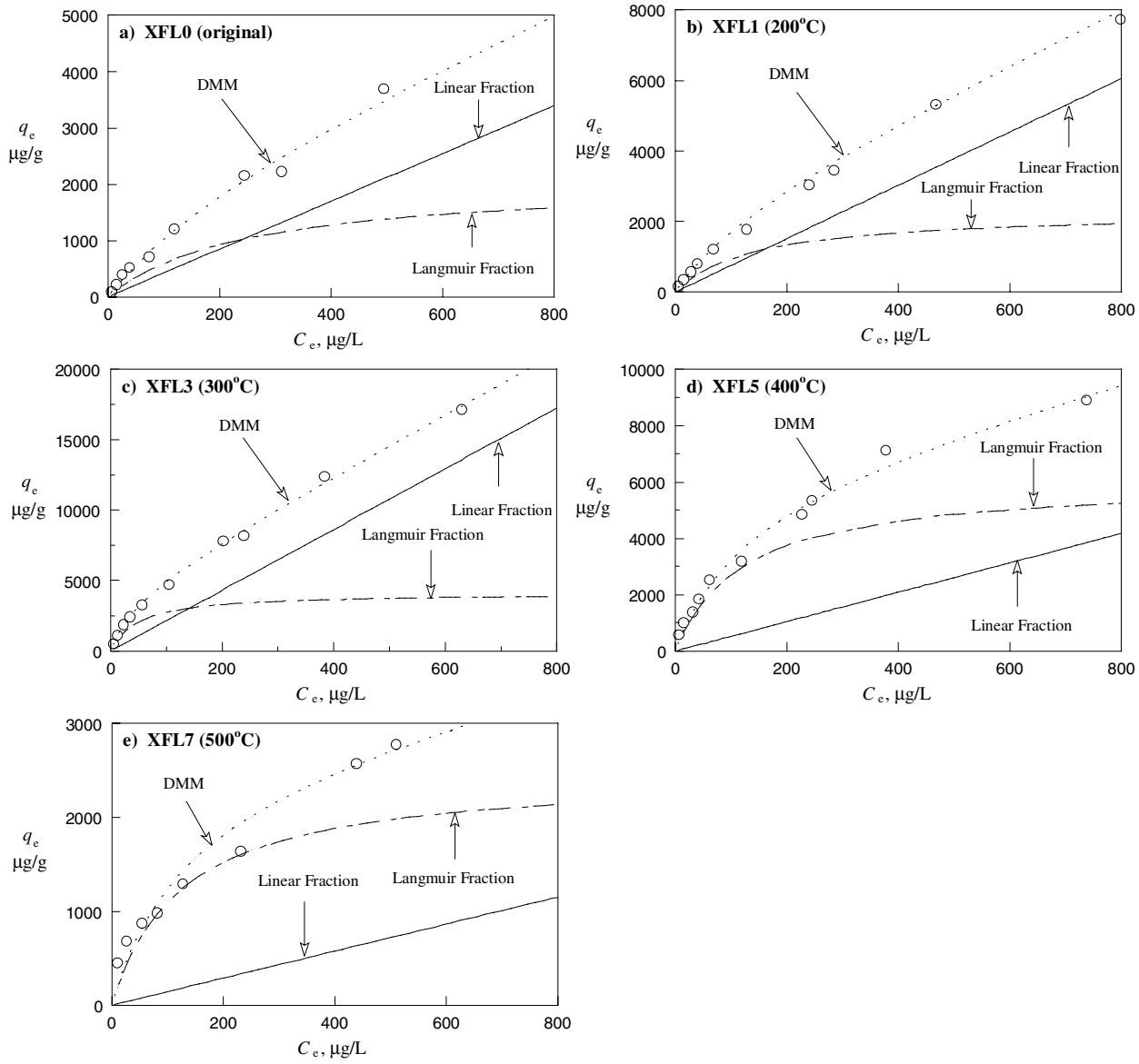


FIGURE SI-2. Fitting of the TCB isotherm data to the Dual Mode Model for five kerogen samples. The empty circles are the measured isotherm data. The solid and broken lines represent respectively the contribution of the linear partition and site-limiting adsorption components to the overall sorption (dotted line) by each kerogen sample.