Supplementary Data

**Comprehending adsorption of methylethylketone and toluene and microwave regeneration effectiveness for beaded activated carbon derived from recycled waste bamboo tar**

Yu-Ting Chen

Graduate Institute of Environmental Engineering, National Taiwan University, No. 1, Sec. 4, Roosevelt Rd., Da'an Dist., Taipei 106, Taiwan

Ying-Pin Huang

Central Region Campus, Industrial Technology Research Institute, No. 8, Gongyan Rd., Liujia Dist., Tainan 734, Taiwan

Can Wang a,b

a School of Environmental Science and Engineering, Tianjin University, Tianjin 300072, China

b Tianjin Key Lab of Indoor Air Environmental Quality Control, Tianjin 300072, China

Ji-Guang Deng

College of Environmental and Energy Engineering, Beijing University of Technology, Beijing, 100124, China.

Hsing-Cheng Hsi\*

Graduate Institute of Environmental Engineering, National Taiwan University, No. 1, Sec. 4, Roosevelt Rd., Da'an Dist., Taipei 106, Taiwan

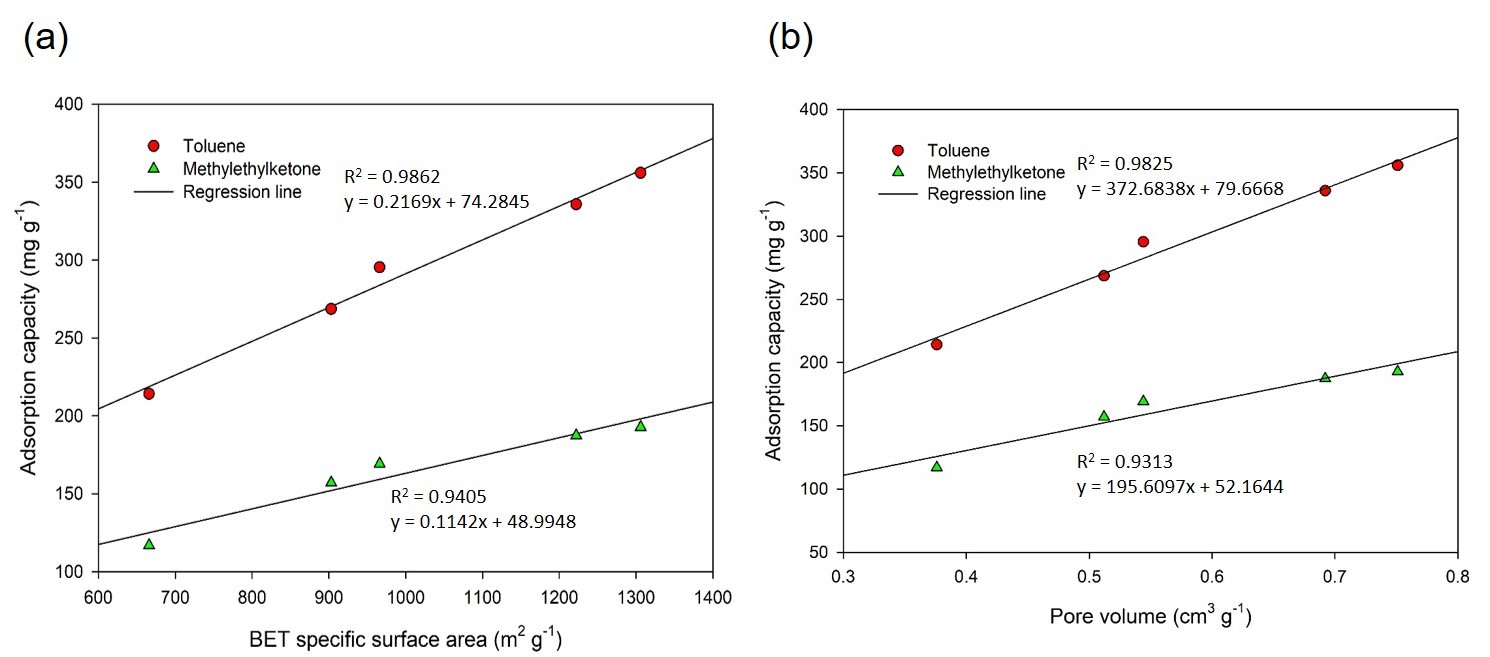
\*Correspondence author:

Tel: +886 2 33664374; fax: +886 2 23928830.

E-mail address: hchsi@ntu.edu.tw (H.-C. Hsi)

Graduate Institute of Environmental Engineering, National Taiwan University

No. 1, Sec. 4, Roosevelt Rd., Da’an Dist., Taipei 106, Taiwan

****

**Figure S1.** Relationships between (a) BET specific surface area and (b) pore volume and adsorption capacities.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table S1.** Langmuir parameters for MEK and toluene adsorption onto bamboo-tar-derived and commercial BAC. | | | | | |
| Langmuir parameter | | | | | |
| Adsorbate | Adsorbent | Temperature (°C) | R2 | qs (mg g-1) | b |
| MEK | SBAC-T900-t3 | 30 | 0.999 | 408.6 | 124.8 |
|  |  | 40 | 0.997 | 360.0 | 146.9 |
|  |  | 50 | 0.997 | 322.2 | 180.2 |
|  | SBAC-T900-t4 | 30 | 0.999 | 483.8 | 114.3 |
|  |  | 40 | 0.998 | 421.3 | 129.1 |
|  |  | 50 | 0.986 | 357.0 | 148.9 |
|  | KBAC | 30 | 0.999 | 373.5 | 283.1 |
|  |  | 40 | 0.999 | 361.3 | 282.9 |
|  |  | 50 | 0.998 | 333.9 | 275.9 |
| TOL | SBAC-T900-t3 | 30 | 0.997 | 471.8 | 124.4 |
|  |  | 40 | 0.998 | 443.1 | 186.6 |
|  |  | 50 | 0.993 | 397.2 | 233.4 |
|  | SBAC-T900-t4 | 30 | 0.999 | 552.2 | 139.4 |
|  |  | 40 | 0.998 | 501.7 | 188.0 |
|  |  | 50 | 0.995 | 463.1 | 206.0 |
|  | KBAC | 30 | 0.999 | 412.3 | 476.5 |
|  |  | 40 | 0.999 | 398.3 | 417.5 |
|  |  | 50 | 0.999 | 387.2 | 472.1 |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table S2.** Freundlich parameters for MEK and toluene adsorption onto bamboo-tar-derived and commercial BAC. | | | | | |
| Freundlich parameter | | | | | |
| Adsorbate | Adsorbent | Temperature (°C) | R2 | *K* | *n*F |
| MEK | SBAC-T900-t3 | 30 | 0.934 | 618.5 | 4.57 |
|  |  | 40 | 0.974 | 618.3 | 4.05 |
|  |  | 50 | 0.976 | 696.3 | 3.39 |
|  | SBAC-T900-t4 | 30 | 0.939 | 758.6 | 4.23 |
|  |  | 40 | 0.981 | 762.5 | 3.67 |
|  |  | 50 | 0.959 | 769.2 | 3.24 |
|  | KBAC | 30 | 0.915 | 502.9 | 7.28 |
|  |  | 40 | 0.943 | 561.3 | 5.50 |
|  |  | 50 | 0.916 | 650.2 | 4.18 |
| TOL | SBAC-T900-t3 | 30 | 0.971 | 537.9 | 8.89 |
|  |  | 40 | 0.977 | 597.5 | 6.39 |
|  |  | 50 | 0.942 | 567.6 | 6.20 |
|  | SBAC-T900-t4 | 30 | 0.980 | 686.4 | 6.89 |
|  |  | 40 | 0.978 | 693.9 | 6.04 |
|  |  | 50 | 0.957 | 639.6 | 6.29 |
|  | KBAC | 30 | 0.943 | 443.5 | 20.96 |
|  |  | 40 | 0.951 | 446.5 | 15.78 |
|  |  | 50 | 0.964 | 468.1 | 11.44 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Table S3.** D-R parameters for MEK and toluene adsorption onto bamboo-tar-derived and commercial BAC. | | | | | | | |
| D-R parameter | | | | | | | |
| Adsorbate | Adsorbent | Temperature  (°C) | R2 | *W*0  (cm3 g-1) | *E*0  (KJ mol-1) | *E*  (KJ mol-1) | *x*0  (nm) |
| MEK | SBAC-T900-t3 | 30 | 0.983 | 0.5595 | 14.72 | 14.25 | 0.825 |
| 40 | 0.999 | 0.5032 | 15.49 | 15.02 | 0.775 |
| 50 | 0.995 | 0.4915 | 15.34 | 14.89 | 0.782 |
| SBAC-T900-t4 | 30 | 0.985 | 0.6665 | 14.64 | 14.18 | 0.820 |
| 40 | 0.993 | 0.5904 | 14.77 | 14.32 | 0.812 |
| 50 | 0.977 | 0.5291 | 14.49 | 14.07 | 0.828 |
| KBAC | 30 | 0.981 | 0.5116 | 18.91 | 18.31 | 0.635 |
| 40 | 0.990 | 0.5156 | 17.98 | 17.43 | 0.667 |
| 50 | 0.966 | 0.5182 | 16.90 | 16.41 | 0.710 |
| Toluene | SBAC-T900-t3 | 30 | 0.943 | 0.5345 | 17.01 | 20.28 | 0.705 |
| 40 | 0.992 | 0.5410 | 15.39 | 18.35 | 0.780 |
| 50 | 0.947 | 0.4952 | 15.98 | 19.06 | 0.751 |
| SBAC-T900-t4 | 30 | 0.996 | 0.6537 | 14.42 | 17.20 | 0.832 |
| 40 | 0.994 | 0.6199 | 14.90 | 17.77 | 0.805 |
| 50 | 0.945 | 0.5623 | 16.60 | 19.80 | 0.723 |
| KBAC | 30 | 0.988 | 0.4896 | 23.35 | 27.84 | 0.514 |
| 40 | 0.991 | 0.4801 | 22.34 | 26.64 | 0.537 |
| 50 | 0.992 | 0.4823 | 20.96 | 24.99 | 0.573 |

**Determining isosteric heat of adsorption using Dubinin-Radushkevich and Clausius-Clapeyron equations**

The heat of adsorption, Δ*H*s, can be determined by two established ways: direct measurements using adsorption calorimetry or indirect calculations through adsorption isotherm data at various temperatures (Builes et al., 2013; Whittaker et al., 2013). In deriving equations and analytical solutions to obtain Δ*H*s, we followed the procedures developed by Qi et al. (2000) and Ramirez et al. (2005), which are shown below.

In conventional approaches, one considers the variation of adsorbate partial pressure, *P*, with temperature, *T*, at a fixed loading, *q*, to obtain Δ*H*s. However, combining the Clausius-Clapeyron (C-C) equation with Polanyi-potential-derived isotherms such as the Dubinin-Radushkevich (D-R) isotherm can result in an analytical solution of Δ*H*s. The C-C equation is expressed as:

|  |  |  |
| --- | --- | --- |
|  |  | (S1) |

The D-R equation, which expresses the adsorption capacity as a function of adsorption potential is as follows:

|  |  |  |
| --- | --- | --- |
|  |  | (S2) |

and

|  |  |  |
| --- | --- | --- |
|  |  | (S3) |

Substituting the Polanyi’s (adsorption) potential, *ε*, into the C-C equation yields:

|  |  |  |
| --- | --- | --- |
|  |  | (S4) |

where Δ*H*s equals to the summation of three types of energy during the adsorption processes: the heat of vaporization, the adsorption potential, and the change of maximum adsorption capacity with temperature (Ramirez et al., 2005).

The last term on the right hand side can be modified and equation S4 becomes:

|  |  |  |
| --- | --- | --- |
|  |  | (S5) |

The thermal expansion coefficient, *α*, is expressed as:

|  |  |  |
| --- | --- | --- |
|  |  | (S6) |

where *ρ*b and *ρ*c are saturated liquid densities at normal boiling temperature (*T*b) and critical temperature (*T*c) obtained from Poling et al. (2001).

Assuming the temperature-independency of *ε*, equation S5 becomes:

|  |  |  |
| --- | --- | --- |
|  |  | (S7) |

Equation S3 can be rewritten as:

|  |  |  |
| --- | --- | --- |
|  |  | (S8) |

Substituting equation S8 into equation S7, we obtain:

|  |  |  |
| --- | --- | --- |
|  |  | (S9) |

The heat of vaporization term can be calculated based upon Wagner liquid-vapor pressure equation (Ramirez et al., 2005):

|  |  |
| --- | --- |
|  | (S10) |

where *a*1 – *a*4 are Wagner constants and x = (1 – *T*/*T*c).

The above-mentioned thermodynamic parameters are listed in Table S1

**Table S1.** Parameters used in calculating isosteric heat of adsorption.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Adsorbate | *T*b (K) | *T*c (K) | *ρ*b (g cm-3) | *ρ*c (g cm-3) | *α* (K-1) | Wagner constanta | | | |
| *a*1 | *a*2 | *a*3 | *a*4 |
| MEK | 352.71 | 536.80 | 0.742 | 0.270 | 0.00168 | -7.6642 | 1.7175 | -2.0991 | -4.5861 |
| TOL | 383.79 | 591.75 | 0.779 | 0.294 | 0.00113 | -7.4183 | 1.8401 | -2.1458 | -3.7081 |

a Forero and Velasquez (2011)

**References**

1. Builes, S., S.I. Sandler, and R.C. Xiong. 2013. Isosteric heats of gas and liquid adsorption. *Langmuir* 29(33):10416-10422.
2. Forero, L.A., and J.A. Velasquez. 2011. Wagner liquid-vapour pressure equation constants from a simple methodology. *J. Chem. Thermodyn.* 43(8):1235-1251.
3. Poling, B.E., J.M. Prausnitz, and J.P. O'Connell. 2001. The properties of gases and liquids, fifth ed. Mcgraw-hill, New York.
4. Qi, S.Y., K.J. Hay, M.J. Rood, and M.P. Cal. 2000. Equilibrium and heat of adsorption for water vapor and activated carbon. *J. Environ. Eng.-ASCE* 126(3):267-271.
5. Ramirez, D., S.Y. Qi, and M.J. Rood. 2005. Equilibrium and heat of adsorption for organic vapors and activated carbons. *Environ. Sci. Technol.* 39(15):5864-5871.
6. Whittaker, P.B., X.L. Wang, K. Regenauer-Lieb, and H.T. Chua. 2013. Predicting isosteric heats for gas adsorption. *Phys. Chem. Chem. Phys.* 15(2):473-482.