**Supplementary material for**

# Sorption of perfluorooctane sulfonate and perfluorooctanoate on Polyacrylonitrile fibers-derived activated carbon fibers: In comparison with activated carbon

**Wei Chen [a, b, c], Xiaoping Zhang [a, b, c *], Mairambek Mamadiev [a, b, c], Zihao Wang [a, b, c]**

[a] School of Environment and Energy, South China University of Technology, Guangzhou Higher Education Mega Centre, Guangzhou 510006, PR China

[b] The Key Lab of Pollution Control and Ecosystem Restoration in Industry Clusters, Ministry of Education, South China University of Technology, Guangzhou Higher Education Mega Centre, Guangzhou 510006, PR China

[c] Guangdong Environmental Protection Key Laboratory of Solid Waste Treatment and Recycling, South China University of Technology, Guangzhou Higher Education Mega Centre, Guangzhou 510006, PR China

*Corresponding author at: School of Environment and Energy, South China University of Technology, Guangzhou 510006, China. Tel.: +86 20 39380569

E-mail addresses: xpzhang@scut.edu.cn.

**Table 1** Characteristic parameters of polyacrylonitrile fibers (PANFs)

| | PANFs |
|---|---|
| Average diameter (μm) | 17.05 |
| Tensile strength (eN/dtex) | 4.5 |
| Elongation at break point (%) | 16-19 |
| Density (g/cm$^3$) | 1.19 |
| Linear density (dtex) | 1.12-1.33 |
| Carbon content (%) | 65 |
| Moisture content (%) | 0.6-0.9 |
| Melting point ($^o$C) | 317 |

**Table 2** Characteristic parameters of PANFs-derived PACFs

| | PANFs |
|---|---|
| Specific surface areas (m$^2$/g) | 1781.59 |
| Average diameter (μm) | 12.27 |
| Total pore volume (cm$^3$/g) | 0.94 |
| Carbon content (%) | 82 |
| Ash yield (%) | 2-3 |
| The loss of mass on drying method | 35 |

## Sorption kinetics models

Pseudo-first-order and pseudo-second-order kinetics equations are represented as the functions of $q_t$, $q_e$ and $t$, which are given as below [1]:

Pseudo-first-order model:

$$\lg(q_e - q_t) = \lg q_e - \frac{k_1}{2.303} t \quad (3)$$

Pseudo-second-order model:

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^{\,2}} + \frac{1}{q_e} t = \frac{1}{v_0} + \frac{t}{q_e} \quad (4)$$

Where $k_1$ (1/h) and $k_2$ (g/mmol//h) are the sorption rate constants of the pseudo-first-order model and the pseudo-second-order model, respectively. $v_0$ is the initial adsorption rate (mmol/h/g). Other parameters are defined in equation (1).

**Intra-particle diffusion and Boy's film-diffusion models**

The intra-particle diffusion model is shown as below [2]:

$$q_t = K_i t^{0.5} + C_i \qquad (5)$$

Where $K_i$ is the intra-particle diffusion rate constant (mmol/g·h$^{1/2}$) at stage i and $C_i$ is the intercept corresponding to stage i, which is proportional to the boundary layer thickness. The values of $K_i$ and $C_i$ can be evaluated from the linear plots of $q_t$ versus $t^{1/2}$.

The Boy's film-diffusion model is shown as below [3]:

$$F = 1 - \left(\frac{6}{\pi^2}\right)\exp(-B_t) \qquad (6)$$

Where $F$ is the fractional attainment of equilibrium at different t (h), and $B_t$ is a mathematical function of F.

$$F = \frac{q_e}{q_e} \qquad (7)$$

$$B_t = -0.4977 - \ln(1 - F) \qquad (8)$$

Where $B_t$ can be calculated from equation (8) according to each value of F. The linearity of this plot provides a reliable information to identify that the rates of sorption is controlled by external mass transfer (film diffusion) or intraparticle diffusion.

**Sorption isotherm models**

The Langmuir and Freundlich model equations are given as below [4]:

Langmuir model:

$$q_e = \frac{bq_m C_e}{1 + bC_e} \qquad (9)$$

Freundlich model:

$$q_e = K_F C_e^{\,n} \qquad (10)$$

Where $C_e$ (mmol/L) and $q_e$ (mmol/g) are the concentration of PFOS/PFOA in water and adsorbed on adsorbent reaching adsorption equilibrium, respectively. $K_F$ and $n$ are Freundlich constants related to adsorption capacity and adsorption intensity of the adsorbents, respectively. $q_m$ (mmol/g) is the maximum sorption capacity, and $b$ is the sorption equilibrium constant of Langmuir model related to the affinity of binding sites.

**Sorption site energy distributions**

The approximate site energy distributions underlying Freundlich isotherm was introduced to relate the differences in sorption isotherms to alteration of energetic characteristics of different adsorbates-adsorbents interactions. It was based on the assumption of condensation approximation and expressed by the following equation (11) [5].

$$\phi(\varepsilon) = \frac{K_F \cdot n \cdot S_W^n}{RT} \exp\left(\frac{-n\varepsilon}{RT}\right) \qquad (11)$$

In the equation, ε is the net energy that equals to $E_{total}$-$E_S$, where $E_{total}$ is the difference of sorption energy to a given site between adsorbate and water, $S_W$ is the water solubility of the adsorbate, and $E_S$ is the sorption energy at $C_e$= $S_W$. R is the universal gas constant, and T is the absolute temperature. Other parameters are defined in equation (10).

**References**


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