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)

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>PANFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average diameter (μm)</td>
<td>17.05</td>
</tr>
<tr>
<td>Tensile strength (eN/dtex)</td>
<td>4.5</td>
</tr>
<tr>
<td>Elongation at break point (%)</td>
<td>16-19</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>1.19</td>
</tr>
<tr>
<td>Linear density (dtex)</td>
<td>1.12-1.33</td>
</tr>
<tr>
<td>Carbon content (%)</td>
<td>65</td>
</tr>
<tr>
<td>Moisture content (%)</td>
<td>0.6-0.9</td>
</tr>
<tr>
<td>Melting point (°C)</td>
<td>317</td>
</tr>
</tbody>
</table>

Table 2 Characteristic parameters of PANFs-derived PACFs

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>PANFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific surface areas (m²/g)</td>
<td>1781.59</td>
</tr>
<tr>
<td>Average diameter (μm)</td>
<td>12.27</td>
</tr>
<tr>
<td>Total pore volume (cm³/g)</td>
<td>0.94</td>
</tr>
<tr>
<td>Carbon content (%)</td>
<td>82</td>
</tr>
<tr>
<td>Ash yield (%)</td>
<td>2-3</td>
</tr>
<tr>
<td>The loss of mass on drying method</td>
<td>35</td>
</tr>
</tbody>
</table>

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:

\[
\lg(q_e - q_t) = \frac{k_1}{2.303} \frac{1}{q_e} t
\]  (3)

Pseudo-second-order model:

\[
\frac{t}{q_t} = \frac{1}{k_2 q_e} + \frac{1}{q_e} + \frac{t}{v_0 q_e}
\]  (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:

\[
q_i = K_i t^{0.5} + C_i
\]  \hspace{1cm} (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 \(q_i\) versus \(t^{1/2}\).

The Boy’s film-diffusion model is shown as below ³:

\[
F = 1 - \left( \frac{6}{\pi^2} \right) \exp(-B_t) \]  \hspace{1cm} (6)

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

\[
F = \frac{q_e}{q_e} \]  \hspace{1cm} (7)

\[
B_t = -0.4977 - \ln(1 - F) \]  \hspace{1cm} (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:

\[
q_e = \frac{b q_m C_e}{1 + b C_e} \]  \hspace{1cm} (9)
Freundlich model:

\[ q_e = K_F C_e^n \]  \hspace{1cm} (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) \(^5\).

\[ \phi(\varepsilon) = \frac{K_F \cdot n \cdot S_w^n}{RT} \exp\left(\frac{-n\varepsilon}{RT}\right) \]  \hspace{1cm} (11)

In the equation, \( \varepsilon \) is the net energy that equals to \( E_{\text{total}}-E_S \), where \( E_{\text{total}} \) 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**

