Distribution of iron in activated carbon composites:
assessment of arsenic removal behavior

**SORPTION ISOTHERM**

Freundlich isotherm

The Freundlich isotherm, which assumes a heterogeneous surface with a non-uniform distribution of sorption energy, is presented in Equation (S1).

\[ q_e = k_f c_e^{1/n} \]  

(S1)

Here, \( q_e \) (mg g\(^{-1}\)) is adsorbed mass at equilibrium concentration where \( c_e \) (mg L\(^{-1}\)) is the equilibrium concentration and \( k_f \) (mg g\(^{-1}\)(mg L\(^{-1}\))\(^{-1/n}\)) and \( 1/n \) are Freundlich sorption constants. In this equation, when \( n \) is 1, the Freundlich isotherm becomes linear.

Langmuir isotherm

The basic assumptions of Langmuir isotherm (Equation (S2)) are the existence of homogeneous adsorbent surface, monolayer sorption, and a constant sorption potential.

\[ q_e = \frac{q_m k_f c_e}{1 + k_f c_e} \]  

(S2)

Figure S1  
(a) SEM image of the composite AC-Fe(B6) and (b) EDX spectra analyzed on the surface of the same composite (with arsenic sorption). (c) Distribution of relative percentage of iron (at.%) evaluated from EDX analysis in AC-Fe composites (B1 and B6) and (d) XRD analysis of unmodified AC, AC-Fe composites containing highest (B6) and lowest iron (B1).
Here, $q_m$ (mg g$^{-1}$) and $k_t$ (L mg$^{-1}$) are Langmuir sorption constants. Gibbs free energy, $\Delta G$ (kJ mol$^{-1}$), released due to sorption of As ions on the adsorbent surface, was calculated based on the relation $\Delta G = -RT \ln k$. Here $k$ the is sorption constant ($k_f$ or $k_i$) (Kanel et al. 2005). We have considered Langmuir constant $k_l$ in calculating Gibbs free energy. $R$ (8.314 $\times$ 10$^{-3}$ kJ mol$^{-1}$ K$^{-1}$) is the ideal gas constant and $T$ is temperature (K).

**SORPTION KINETICS**

Pseudo first-order, pseudo second-order sorption kinetics models, and Webber Morris model as described using Equations (S3), (S4) and (S5) (Ho & McKay 2000; Argun et al. 2007; Vitela-Rodriguez & Rangel-Mendez 2013).

**Pseudo first-order equation**

$$q_t = q_e(1 - e^{-k_t t})$$

**Pseudo second-order equation**

$$\frac{t}{q_t} = \frac{1}{k'_t q_e^2} + \frac{t}{q_e}$$

**Webber Morris model**

$$q_t = k'' t + C$$

Here, $q_t$ (mg g$^{-1}$) and $q_e$ (mg g$^{-1}$) are the adsorbed mass at time, $t$ (min) and at equilibrium concentration, respectively. $k_t$ (min$^{-1}$) and $k'_t$ (g mg$^{-1}$ min$^{-1}$) are the rate constants for the first-order and second-order sorption kinetics respectively, where, $k''$ (mg g$^{-1}$ min$^{-0.5}$) is the intraparticle diffusion rate constant. $C$ is the y-axis intercept.
Table S1 | Characterization of AC-Fe composites and their arsenic removal efficiency

<table>
<thead>
<tr>
<th>Composites</th>
<th>Initial Fe concentration (molarity)</th>
<th>Final Fe content (wt.%)</th>
<th>BET (m²/g)</th>
<th>Percentage removed, As(V)</th>
<th>Percentage removed, As(III)</th>
<th>Sorption [mg As(V) /gFe]</th>
<th>Sorption [mg As(III) /gFe]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC</td>
<td>0.00</td>
<td>&lt;0.1</td>
<td>582 ± 22.2</td>
<td>19.3</td>
<td>17.1</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>AC-Fe(B1)</td>
<td>0.09</td>
<td>1.54</td>
<td>614 ± 14.3</td>
<td>94.5</td>
<td>42.3</td>
<td>55.4 ± 1.2</td>
<td>23.8 ± 1.1</td>
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<tr>
<td>AC-Fe(B2)</td>
<td>0.18</td>
<td>2.96</td>
<td>574 ± 20.7</td>
<td>98.7</td>
<td>61.6</td>
<td>24.5 ± 0.5</td>
<td>19.0 ± 1.2</td>
</tr>
<tr>
<td>AC-Fe(B3)</td>
<td>0.30</td>
<td>3.87</td>
<td>542 ± 17.3</td>
<td>97.0</td>
<td>59.6</td>
<td>19.7 ± 1.5</td>
<td>12.2 ± 0.9</td>
</tr>
<tr>
<td>AC-Fe(B4)</td>
<td>0.90</td>
<td>4.55</td>
<td>542 ± 20.4</td>
<td>98.2</td>
<td>45.7</td>
<td>17.1 ± 1.2</td>
<td>8.8 ± 1.9</td>
</tr>
<tr>
<td>AC-Fe(B5)</td>
<td>1.80</td>
<td>5.20</td>
<td>530 ± 26.5</td>
<td>98.1</td>
<td>55.2</td>
<td>13.5 ± 2.0</td>
<td>9.2 ± 2.1</td>
</tr>
<tr>
<td>AC-Fe(B6)</td>
<td>3.00</td>
<td>6.01</td>
<td>529 ± 14.2</td>
<td>93.7</td>
<td>56.1</td>
<td>11.5 ± 3.2</td>
<td>7.9 ± 2.3</td>
</tr>
</tbody>
</table>

REFERENCES


