Electronic Supplementary Material (ESI) for RSC Advances.




Supplementary Information

# Electrospun poly(acrylic acid)/poly(vinyl alcohol) nanofibrous adsorbents for Cu(II) removal from industrial plating wastewater

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**Nomenclature**

| | |
|---|---|
| $A$ | modified dose–response model constant |
| $a$ | adsorbent dose |
| $a_n$ | apparent density of the nanofibrous adsorbents |
| $a_R$ | Redlich-Peterson constant |
| $b_n$ | bulk density of the polymer solution |
| $C_{cap}$ | removal capacity of the nanofibrous adsorbents |
| $C_e$ | equilibrium concentration of contaminant in the aqueous solution |
| $C_i$ | initial concentration of contaminant in the aqueous solution |
| $C_0$ | influent concentration into the fixed-bed column |
| $C_v$ | effluent concentration at the filtrate volume $v$ |
| $g$ | Redlich-Peterson constant |
| $\Delta G^0$ | change in Gibb's free energy |
| $\Delta H^0$ | change in enthalpy |
| $K_d$ | distribution coefficient |
| $K_F$ | Freundlich constant |
| $K_L$ | Langmuir constant |
| $K_R$ | Redlich-Peterson constant |
| $K_e$ | equilibrium constant (dimensionless) |
| $k_1$ | pseudo first-order rate constant |
| $k_2$ | pseudo second-order rate constant |
| $1/n$ | Freundlich constant |
| $M_f$ | mass of the nanofibrous adsorbents used in the filtration experiment |

| | |
|---|---|
| $Q_m$ | maximum adsorption capacity |
| $q_{a,exp}$ | mass of contaminant removed per unit mass of the nanofibrous adsorbents |
| $q_e$ | amount of contaminant adsorbed (adsorption capacity) at equilibrium |
| $q_t$ | amount of contaminant adsorbed (adsorption capacity) at time *t* |
| $R$ | gas constant |
| $R^2$ | determination coefficient |
| $S$ | selectivity coefficient |
| SAE | sum of absolute error |
| $\Delta S^0$ | change in entropy |
| V | filtrate volume |
| $V_{total}$ | total filtrate volume |
| $y_c$ | calculated removal capacity from the model |
| $y_e$ | measured removal capacity from the experiment, |
| $y_e$ | average of the measured removal capacity |
| $\alpha$ | initial adsorption rate constant |
| $\beta$ | Elovich adsorption constant |
| $\chi^2$ | chi-square coefficient |

*1. Batch data analysis*

Kinetic models:

$$q_t = q_e\left(1 - e^{-k_1 t}\right), \quad \text{pseudo first-order} \tag{S1}$$

$$q_t = k_2 {q_e}^2 t/(1 + k_2 q_e t), \quad \text{pseudo second-order} \tag{S2}$$

$$q_t = \ln(\alpha\beta)/\beta + \ln t/\beta \quad \text{Elovich} \tag{S3}$$

Thermodynamic models:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0, \tag{S4}$$

$$\Delta G^0 = -RT ln K_e;\ K_e = \frac{aq_e}{C_e}, \tag{S5}$$

$$\ln(K_e) = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT}, \tag{S6}$$

Equilibrium isotherm models:

$$q_e = \frac{Q_m K_L C_e}{1 + K_L C_e}, \quad Langmuir \tag{S7}$$

$$q_e = K_F {C_e}^{1/n}, \quad Freundlich \tag{S8}$$

$$q_e = \frac{K_R C_e}{1 + a_R {C_e}^g}, \quad Redlich - Peterson \tag{S9}$$

In order to obtain parameter values from the models, nonlinear regression was performed using $R^2$, $\chi^2$, and *SAE* as follows:

$$R^2 = \sum_{i=1}^{m}(y_c - \bar{y}_e)_i^2 \left[\sum_{i=1}^{m}(y_c - \bar{y}_e)_i^2 + \sum_{i=1}^{m}(y_c - y_e)_i^2\right] \quad \text{(S10)}$$

$$\chi^2 = \left[(y_e - y_c)^2/y_c\right]_i \quad \text{(S11)}$$

$$SAE = \sum_{i=1}^{n}|y_c - y_e|_i \quad \text{(S12)}$$

*2. Filtration data analysis*

The total mass of Cu(II) injected into the nanofibers during the experiment ($M_{total}$) was calculated as follows:

$$M_{total} = C_0 V_{total}, \quad \text{(S13)}$$

The Cu(II) removal capacity of the nanofibers ($C_{cap}$) was quantified as follows:

$$C_{cap} = \int_{V=0}^{V=V_{total}} (C_0 - C_V)\, dt, \quad \text{(S14)}$$

The mass of Cu(II) removed per unit mass of the nanofibers ($q_{a,exp}$) was determined as follows:

$$q_{a,exp} = C_{cap}/M_f, \quad \text{(S15)}$$

The modified dose-response model was used to analyze the filtration data as follows:

$$\frac{C_V}{C_0} = 1 - \frac{1}{\left(\frac{C_0 V}{q_{a,mod} M_f}\right)^A + 1} \quad \text{(S16)}$$

**Table S1.**

Kinetic model parameters determined from the experimental data

| Temp. | Pseudo first-order | | | | | Pseudo second-order | | | | | Elovich | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| (°C) | $q_e$ (mg/g) | $k_1$ (/h) | $R^2$ | *SAE* | $\chi^2$ | $q_e$ (mg/g) | $k_2$ (g/mg/ h) | $R^2$ | *SAE* | $\chi^2$ | $\alpha$ (mg/g/h) | $\beta$ (g/mg) | $R^2$ | *SAE* | $\chi^2$ |
| 15 | 18.5 | 0.25 | 0.94 | 7.90 | 5.03 | 20.9 | 0.02 | 0.96 | 6.41 | 2.09 | 19.9 | 0.27 | 0.96 | 4.63 | 0.86 |
| 30 | 44.9 | 1.12 | 0.81 | 18.01 | 4.57 | 48.3 | 0.03 | 0.76 | 24.17 | 4.91 | 512.4 | 0.14 | 0.59 | 38.54 | 8.13 |
| 45 | 45.6 | 1.34 | 0.95 | 11.47 | 0.77 | 50.7 | 0.03 | 0.95 | 11.87 | 1.01 | 556.8 | 0.14 | 0.78 | 25.97 | 3.80 |

**Table S2.**

Equilibrium model parameters determined from the experimental data

| Langmuir | | | | | Freundlich | | | | | Redlich-Peterson | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $q_m$ (mg/g) | $K_L$ (L/mg) | $R^2$ | *SAE* | $\chi^2$ | $K_F$ (L/g) | *1/n* | $R^2$ | *SAE* | $\chi^2$ | *g* | $K_R$ (L/g) | $a_R$ (L/mg) | $R^2$ | *SAE* | $\chi^2$ |
| 49.3 | 0.02 | 0.961 | 10.09 | 1.97 | 12.5 | 0.20 | 0.958 | 11.66 | 2.60 | 0.81 | 156.2 | 13.5 | 0.800 | 16.48 | 6.60 |