Supporting Information

An ultralight aerogel-type urea absorbent for the development of a wearable artificial kidney

Yaping Yuan, ‡[a] Jing Li, ‡[b, *] Chenyuan Guo,[c] Lili Zhang,[a] Yuyan Song,[a] Yanli He,[a]

Yankun Luo[d] and Shuguang Shen [a,*1]

1. Calculation of the Segal crystallinity index

Relative crystallinity of cellulose, was determined using Eq. (1), Eq. (2). [1,2]

$$\text{Cellulose I:} \quad \text{CrI\%} = \frac{I_{(002)} - I_{am}}{I_{(002)}} \times 100 \tag{1}$$

$$\text{Cellulose II:} \quad \text{CrI\%} = \frac{I_{(110)} - I_{am}}{I_{(110)}} \times 100 \tag{2}$$

where $I_{(002)}$ and $I_{(110)}$ are the diffraction intensity of the central crystalline peak (002)

and (110). I_{am} was the diffraction intensity of the amorphous cellulose.

2. Adsorption thermodynamics

[1] [a] College of Chemical Engineering and Technology, Taiyuan University of Technology, Taiyuan 030024, China.

[b] College of Biomedical Engineering, Taiyuan University of Technology, Taiyuan 030024, China.

[c] Shanxi Beifang Xingan Chemical Industry Co., Ltd, Taiyuan 030023, China.

[d] Shanxi Provincial People's Hospital, Taiyuan, China.

* Corresponding author: Shuguang Shen, Jing Li

Corresponding author E-mail: shenshuguang@tyut.edu.cn and sgshen@sina.com

Corresponding Author Address: College of Chemical Engineering and Technology, Taiyuan University of Technology, Taiyuan 030024, China, Tel. (+86) 13303511628.

† Electronic supplementary information (ESI) available: The mechanism of urea adsorption on cellulose aerogels was investigated by adsorption thermodynamics and kinetics. Formulas and any associated references are available in the ESI.

‡ Yaping Yuan and Jing Li contributed equally to this work. Yaping Yuan and Jing Li should be considered co-first authors.

The adsorption processes of cellulose aerogel to urea at 25, 37 and 50 °C were investigated by Langmuir, Freundlich model in the work.

The linear equation of Langmuir model is as follows:

$$\frac{C_e}{q_e} = \frac{1}{K_L q_{max}} + \frac{C_e}{q_{max}} \tag{3}$$

Where q_e is the adsorbed amount of urea in an equilibrium state, mg/g; C_e represents the equilibrium concentration of urea, mg/L; C_0 is the initial concentration of urea, mg/L; K_L represents the adsorption equilibrium constants of the Langmuir model, L/g; q_{max} is the theoretical maximum adsorption capacity of Langmuir models, mg/g.

The linear equation of Freundlich model is given by:

$$\log q_e = \log K_f + \frac{1}{n} \log C_e \tag{4}$$

The "1/n" in the Freundlich isotherm model reflects the intensity of adsorption. If the value of 1/n is less than 0.5 means that the adsorbate is easily adsorbed; while the value more than 2, the adsorption is unfavorable. [3]

Where q_e and C_e are the same as Eq. (3); K_f represents the adsorption equilibrium constants of the Freundlich model, mg/(g·(mg/L)$^{1/n}$);

The Gibb's free energy (ΔG,[4] kJ/mol), adsorption enthalpy (ΔH, kJ/mol) and entropy of adsorption (ΔS, J/(mol·K)) were calculated to better analysis the mechanism of the adsorption process. The formulas are as follows:

$$K = K_f^{n} \tag{5}$$

$$\Delta G = -nRT \tag{6}$$

$$\ln K = -\frac{\Delta H}{RT} + C \tag{7}$$

$$\Delta S = \frac{\Delta H - \Delta G}{T} \tag{8}$$

3. Adsorption kinetics

Kinetic experiments were carried out to study the adsorption behavior of urea by cellulose aerogel. The experimental data were fitted and analyzed by pseudo-first-order kinetic (PFO), pseudo-second-order kinetic (PSO) model.

The equation of PFO is given in the following:

$$\log(q_e\text{-}q_t) = \log(q_e)\text{-}(\frac{k_1 t}{2.303}) \tag{9}$$

The equation of PSO is given in the following:

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \tag{10}$$

where q_e is the adsorbed amount of urea in an equilibrium state, mg/g; q_t is the adsorption capacity at time t, mg/g; k_1 is the rate constant of the PFO model, min^{-1}; k_2 is the rate constant of the PSO model, g/ (mg·min).

The apparent rate constant k_1 was determined from the kinetic experimental data and used to calculate the apparent activation energy. It can be estimated in linear form by the following equation:

$$\ln k = \ln A - \frac{E_a}{RT} \tag{11}$$

where k is the apparent rate constant, min^{-1}; A is the pre-exponential factor, min^{-1}; Ea is the apparent activation energy, kJ/mol.

Since the PFO and PSO model did not provide the information on the diffusion of urea adsorbed by 3CA, an intraparticle diffusion model was used to explain the diffusion mechanism.

$$q_t = K_{id}t^{0.5} + C \qquad (12)$$

where K_{id} is the intraparticle diffusion rate constant, mg/(g·min$^{0.5}$); C is a constant related to the thickness of boundary layer, mg/g.

Notes and references

1   A. Kljun, T. A. Benians, F. Goubet, F. Meulewaeter, J. P. Knox and R. S. Blackburn, *Biomacromolecules*., 2011, **12**, 4121-4126.

2   Y. Xia, X. Li, Y. Yuan, J. Zhuang and W. Wang, *Cellulose*., 2021.

3   S. Fan, Y. Wang, Z. Wang, J. Tang, J. Tang and X. Li, *J. Environ. Chem. Eng*., 2017, **5**, 601-611.

4   F. Xue, F. Wang, S. Chen, S. Ju and W. Xing, *J. Chem. Eng. Data*., 2017, **62**, 4266-4272.