

Supporting Information

for

Rapid and effective preparation of HPEI modified biosorbent based on cellulose fiber with microwave irradiation method for enhanced arsenic removal in water

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Fig. S1 shows the components of the microwave reactor which purchase from PreeKem Scientific Instruments Co., Ltd. The maximum output of the reactor is 1200 W and the temperature was controlled precisely by inserting fiber optic sensor into the solution. In addition, both mechanical and magnetic stirring are available for application.

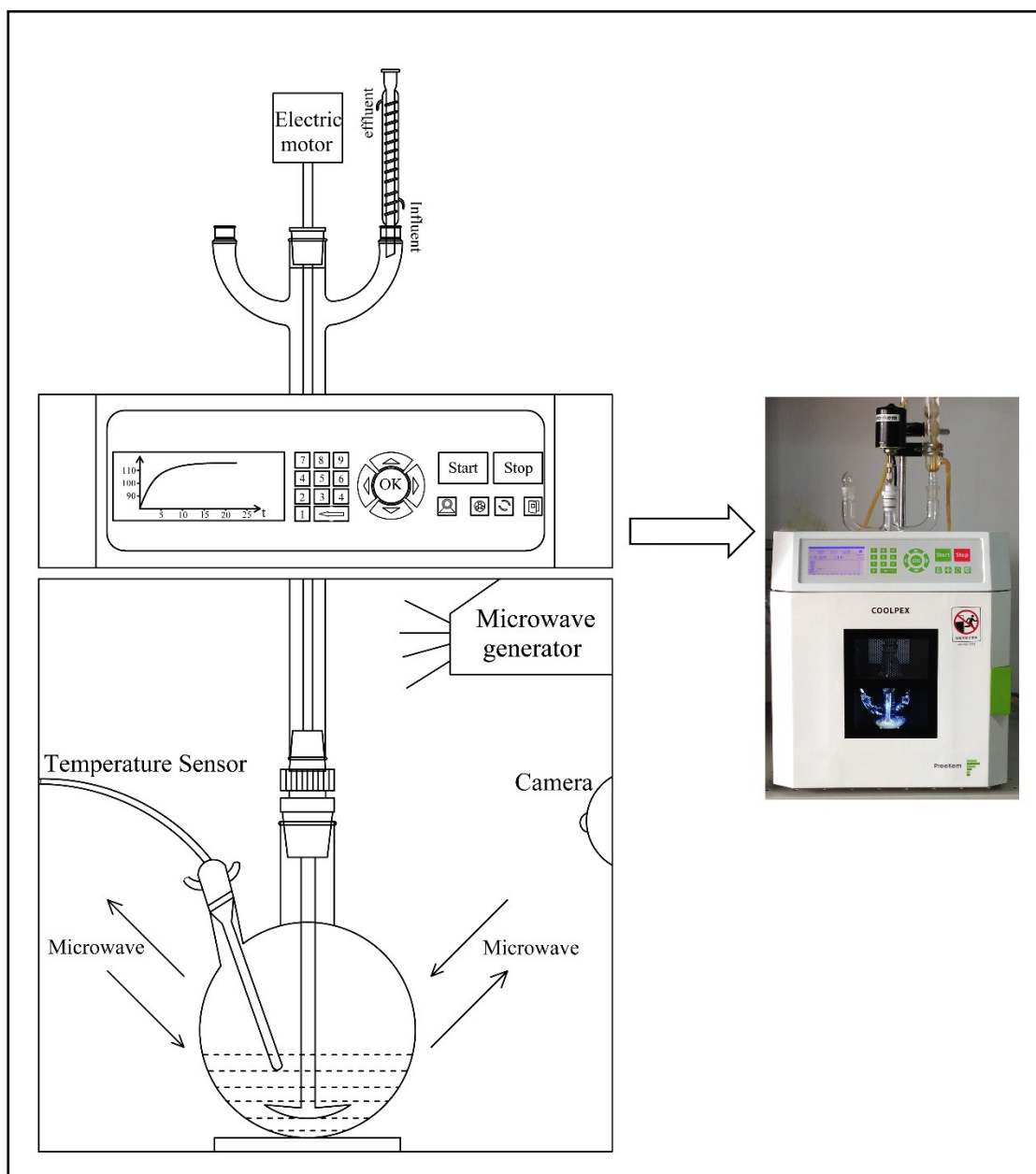


Fig. S1 The feature of the MW reactor (PreeKem Scientific Instruments Co., Ltd.).

Fig. S2 exhibits the effects of reaction temperature and time for the synthesis of Cell_{MW}-ECH fibers and mass ratio of HPEI (wt%) for the preparation of Cell_{MW}-HPEI fiber under MW irradiation.

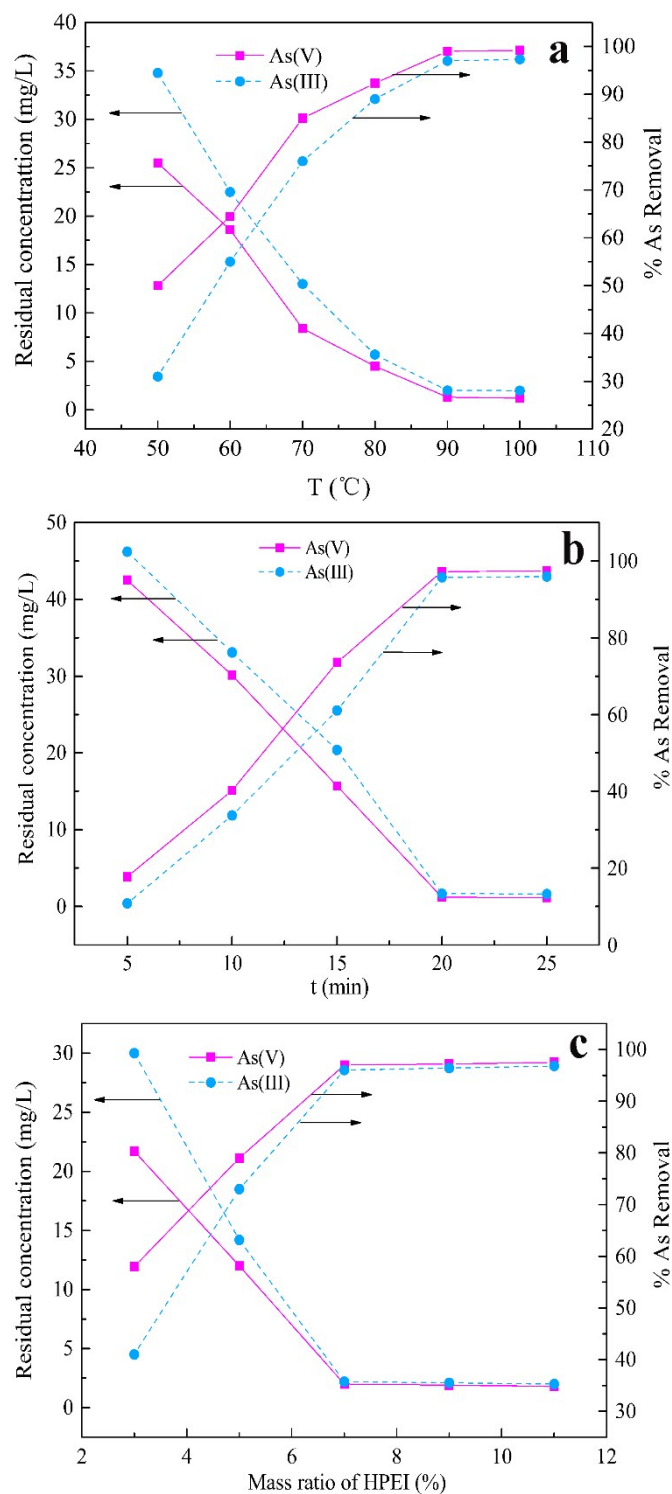


Fig. S2 The residue concentration and the calculated removal efficiency (%) of As(III)/As(V) ions influenced by (a) temperature; (b) reaction time; (c) mass ratio of HPEI (%).

Adsorption Kinetics:

The pseudo-first-order is the Lagergren pseudo-first order rate equation:

$$q_t = q_e (1 - e^{-k_1 t}) \quad (1)$$

where q_e and q_t are the amount of arsenic adsorbed ($\text{mg} \cdot \text{g}^{-1}$) at equilibrium and at time t (min), respectively, while k_1 (min^{-1}) is the rate constants of the pseudo-first-order model.

The pseudo-second-order kinetic rate equation is expressed as:

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

where k_2 ($\text{g} \cdot \text{mg}^{-1} \cdot \text{min}^{-1}$) is the pseudo-second-order rate constant.

The intraparticle diffusion kinetics model of Weber and Morris is represented as follows:

$$q_t = k_3 t^{0.5} + C \quad (3)$$

where, k_3 ($\text{mg} \cdot \text{g}^{-1} \cdot \text{min}^{-1/2}$) is the intraparticle diffusion rate constant and C is the boundary layer thickness.

Typically, these equations are linearized in order that the constants can be found. However, for the sake of reducing error structure and incorrect results in the parameter searching, transformation of linear forms to non-linear kinetic equations were conducted and the data were analyzed by using the following non-linear chi-square test (χ^2):

$$\chi^2 = \sum_{i=1}^n \frac{(q_{e,cal} - q_{e,exp})^2}{q_{e,exp}} \quad (4)$$

where $q_{e,cal}$ ($q_{e,calculated}$) equilibrium capacity obtained by calculated from model ($mg \cdot g^{-1}$) and $q_{e,exp}$. ($q_{e,experimental}$) was the equilibrium capacity from the experimental data ($mg \cdot g^{-1}$). The value of χ^2 calculated from the equation represents the similarity between the data from model and the data from experiment test. A small χ^2 value indicated similarities, while a larger number represents variation of the experimental data.

Adsorption isothermals:

The Langmuir isotherm model is based on the assumption that the adsorbate forms a saturated molecular layer on the adsorbent surface, and the surface sites shares the same energy with no solute-solute or solute-solvent interaction in either phase and transmigration of adsorbate on the plane of the surface. The Langmuir isotherm model can be expressed as:

$$q_e = \frac{q_m K_d C_e}{1 + K_d C_e} \quad (5)$$

where q_e is the amount of metal ion adsorbed at equilibrium by the adsorbent ($\text{mg}\cdot\text{g}^{-1}$), C_e is the equilibrium concentration ($\text{mg}\cdot\text{L}^{-1}$), q_m is theoretical saturation adsorption capacity ($\text{mg}\cdot\text{g}^{-1}$), K_d ($\text{L}\cdot\text{mg}^{-1}$) is the equilibrium Langmuir constant.

Moreover, the dimensionless separation factor R_L could be calculated by applying Langmuir parameters in the following equation:

$$R_L = \frac{1}{1 + K_d C_0} \quad (6)$$

This factor can suggest the favorability of the adsorption process, which was believed to be unfavorable ($R_L > 1$), linear ($R_L = 1$), favorable ($R_L < 1$), or irreversible ($R_L = 0$) at each varies.

The Freundlich isotherms model, which assumes a heterogeneous surface and a multilayer adsorption with an energetic non-uniform distribution, can be expressed as:

$$q_e = K_f C_e^{\frac{1}{n}} \quad (7)$$

where K_f ($\text{mg}\cdot\text{g}^{-1}$) and n are constants representing the adsorption capacity and intensity of adsorption.

The Temkin isotherm model considers that due to adsorbent-adsorbate interactions, the heat of adsorption of all the molecules in the layer would decrease linearly with coverage. Therefore, the adsorbent surface is a uniform distribution of binding energies. The Temkin adsorption isotherm expression is shown as:

$$q_e = \frac{RT}{B_T} \ln(K_T C_e) \quad (8)$$

where K_T ($L \cdot g^{-1}$) is the equilibrium binding constant corresponding to the maximum binding energy, B_T ($kJ \cdot mol^{-1}$) is the Temkin constants relates to the heat of adsorption, R ($8.314 J \cdot mol^{-1} \cdot K^{-1}$) is the universal gas constant and T (K) is the absolute temperature.

$q_{e,cal}$ ($q_{e,calculated}$) was the equilibrium capacity from model ($mg \cdot g^{-1}$) and $q_{e,exp}$ ($q_{e,experimental}$) was the equilibrium capacity obtained from the experimental data ($mg \cdot g^{-1}$).

The thermodynamic parameters ΔG , ΔH and ΔS for this adsorption process were determined by using following equations:

$$\Delta G = -RT \ln K_d \quad (9)$$

$$\ln k = \frac{\Delta S}{R} - \frac{\Delta H}{RT} \quad (10)$$

where K_d is the adsorption equilibrium constant obtained from Langmuir model, R is the universal gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$), T is the temperature (K). The values of ΔH and ΔS could be obtained as the slope and intercept from a linear plot between $\ln k$ versus $1/T$ (Fig. S3, Supporting Information) and the parameters are reported in Table S1.

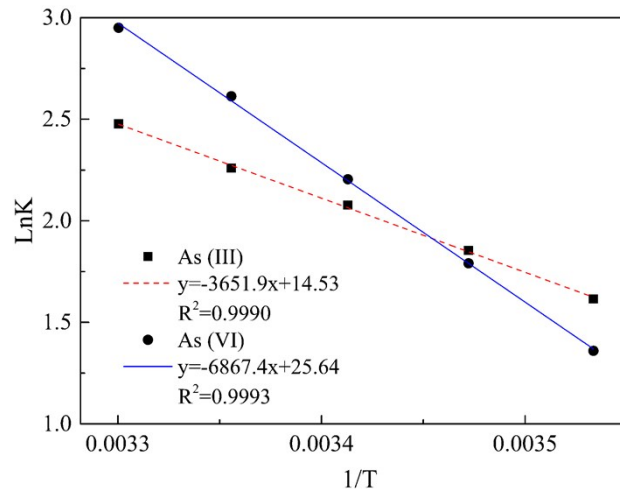


Fig. S3 Thermodynamic study for the adsorption of As(III) and As(V) using Cell_{MW}-HPEI fibers.

Table S1 Thermodynamic parameters for the adsorption of As(III) and As(V) on Cell_{MW}-HPEI.

Metal ions	ΔH (kJ·mol ⁻¹)	ΔS (J·mol ⁻¹ ·k)	ΔG (kJ·mol ⁻¹)				
			283 K	288 K	293 K	298 K	303 K
As (III)	30.26	120.6	-3.80	-4.43	-5.06	-5.60	-6.023
As (V)	57.09	196.5	-3.20	-4.28	-5.37	-6.47	-7.43

Fig. S4 shows the effects of coexisting anions including NO_3^- , Cl^- , SO_4^{2-} , PO_4^{3-} and HA on the adsorption of As(III)/As(V) onto Cell_{MW} -HPEI fibers.

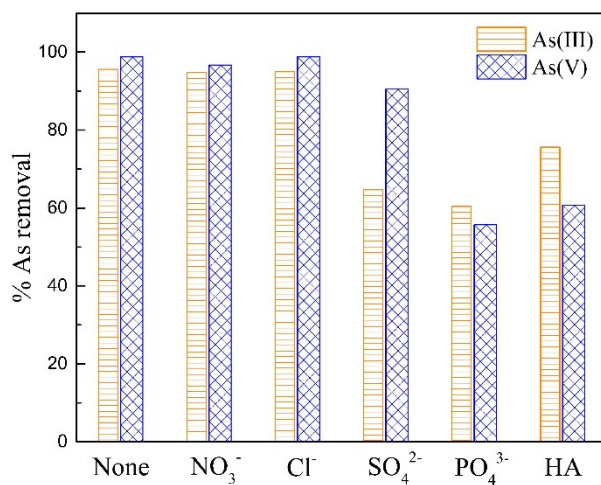


Fig. S4 Effects of coexisting anions and HA on the adsorption of As(III)/As(V) onto Cell_{MW} -HPEI fibers.