Supplementary Materials

Dynamic Adsorption of As(V) onto the Porous α-Fe_2O_3/Fe_3O_4/C Composite Prepared with Bamboo Bio-template

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Table S1. Parameters of the Thomas model and the equilibrium As(V) uptake (q_e) and the total removal percentage (Y) for As(V) adsorption onto PC-Fe/C-B under different conditions.

C_0	Q	Dosage m	Particle size	T	pH	k_{Th}	$q_{e,cal}$	$q_{e,exp}$	Y	R^2
mg/L	mL/min	g	mesh	℃		mL/min·mg	mg/g	mg/g	%	
10	5.136	0.5	<100	35	3	0.00616	13.42	13.29	78.43	0.9877
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
30	5.136	0.5	<100	35	3	0.00306	20.27	19.41	66.33	0.9587
20	4.28	0.5	<100	35	3	0.00334	19.64	19.15	72.18	0.9871
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
20	6.849	0.5	<100	35	3	0.00459	21.61	21	73	0.9779
20	8.561	0.5	<100	35	3	0.00469	20.8	19.34	59.45	0.9368
20	5.136	0.3	<100	35	3	0.00669	17.5	16.88	65.72	0.9801
20	5.136	0.4	<100	35	3	0.00494	20.54	20.19	74.86	0.992
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
20	5.136	0.6	<100	35	3	0.00327	19.71	19.22	72.44	0.989
20	5.136	0.5	60-80	35	3	0.0068	9.61	9.24	69.16	0.9798
20	5.136	0.5	80-100	35	3	0.00421	14.85	14.26	66.12	0.976
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
20	5.136	0.5	<100	25	3	0.0042	18.05	17.6	74.49	0.9756
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
20	5.136	0.5	<100	45	3	0.00419	19.01	18.87	73.48	0.9885
20	5.136	0.5	<100	35	1	0.00384	17.88	17.45	67.94	0.9791
20	5.136	0.5	<100	35	2	0.0041	18.47	18.19	70.84	0.9916
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.00419**	**18.65**	**18.3**	**71.27**	**0.9897**
20	5.136	0.5	<100	35	4	0.00423	16.74	16.42	69.51	0.9902
20	5.136	0.5	<100	35	5	0.00457	14.69	14.27	66.16	0.9779
20	5.136	0.5	<100	35	6	0.00442	12.77	12.37	63.38	0.9862
20	5.136	0.5	<100	35	7	0.0049	7.13	6.68	50.04	0.9456

Note: The subscripts 'exp' and 'calc' show the experimental and calculated values, respectively.

Table S2. Parameters of the Yoon-Nelson model using linear regression analysis for As(V) adsorption onto PC-Fe/C-B under different conditions.

C_0	Q	Dosage m	Particle size	T	pH	k_{YN}	τ_{theo}	τ_{exp}	$\Delta\tau/\tau_{exp}$	$t_{1,theo}$	$t_{1,exp}$	$t_{2,theo}$	$t_{2,exp}$	R^2
mg/L	mL/min	g	mesh	℃		min^{-1}	min	min	%	min	min	min	min	
10	5.136	0.5	<100	35	3	0.0616	131	132	1.06	83	94	166	163	0.9877
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
30	5.136	0.5	<100	35	3	0.0919	66	65	1.22	21	26	90	94	0.9587
20	4.28	0.5	<100	35	3	0.0668	115	110	4.30	60	66	148	152	0.9871
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
20	6.849	0.5	<100	35	3	0.0917	79	75	5.16	39	46	103	105	0.9779
20	8.561	0.5	<100	35	3	0.0938	61	54	12.48	22	26	84	88	0.9368
20	5.136	0.3	<100	35	3	0.1338	51	50	2.20	24	26	68	67	0.9801
20	5.136	0.4	<100	35	3	0.0987	80	79	1.26	43	47	102	103	0.9920
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
20	5.136	0.6	<100	35	3	0.0654	115	111	3.69	59	66	149	151	0.9890
20	5.136	0.5	60-80	35	3	0.1360	47	44	6.33	20	26	63	65	0.9798
20	5.136	0.5	80-100	35	3	0.0841	72	69	4.73	29	32	98	103	0.9760
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
20	5.136	0.5	<100	25	3	0.084	88	89	1.25	44	52	114	115	0.9756
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
20	5.136	0.5	<100	45	3	0.0838	93	92	0.59	49	56	119	118	0.9885
20	5.136	0.5	<100	35	1	0.0767	87	88	1.12	39	47	116	116	0.9791
20	5.136	0.5	<100	35	2	0.0819	90	91	1.20	45	50	117	119	0.9916
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.0838**	**91**	**90**	**0.85**	**47**	**56**	**117**	**117**	**0.9897**
20	5.136	0.5	<100	35	4	0.0845	81	82	0.61	38	43	107	109	0.9902
20	5.136	0.5	<100	35	5	0.0913	72	74	3.37	31	33	96	97	0.9779
20	5.136	0.5	<100	35	6	0.0883	62	61	1.92	21	26	87	90	0.9862
20	5.136	0.5	<100	35	7	0.0979	35	31	12.00	-	6	57	60	0.9456

Note: The subscripts 'exp' and 'calc' show the experimental and calculated values, respectively.

Table S3. Parameters of the Clark model using linear regression analysis for As(V) adsorption onto PC-Fe/C-B under different conditions.

C_0	Q	Dosage m	Particle size	T	pH	r	A	R^2
mg/L	mL/min	g	mesh	℃		mg/L·min	min	
10	5.136	0.5	<100	35	3	0.1781	3.46E+11	0.9786
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
30	5.136	0.5	<100	35	3	0.2435	2.97E+08	0.8689
20	4.28	0.5	<100	35	3	0.1853	6.18E+10	0.9525
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
20	6.849	0.5	<100	35	3	0.2320	2.74E+09	0.9175
20	8.561	0.5	<100	35	3	0.2358	7.29E+07	0.8230
20	5.136	0.3	<100	35	3	0.3383	1.71E+09	0.9047
20	5.136	0.4	<100	35	3	0.2662	6.60E+10	0.9654
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
20	5.136	0.6	<100	35	3	0.1803	3.74E+10	0.9623
20	5.136	0.5	60-80	35	3	0.3724	1.55E+09	0.9486
20	5.136	0.5	80-100	35	3	0.2215	3.18E+08	0.9041
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
20	5.136	0.5	<100	25	3	0.2592	4.09E+11	0.9344
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
20	5.136	0.5	<100	45	3	0.2875	7.94E+13	0.9712
20	5.136	0.5	<100	35	**1**	0.1939	9.06E+08	0.9283
20	5.136	0.5	<100	35	2	0.2139	9.88E+09	0.9527
20	**5.136**	**0.5**	**<100**	**35**	**3**	**0.2214**	**2.42E+10**	**0.9538**
20	5.136	0.5	<100	35	4	0.2274	4.54E+09	0.9424
20	5.136	0.5	<100	35	5	0.2514	2.74E+09	0.9122
20	5.136	0.5	<100	35	6	0.2303	6.79E+07	0.9237
20	5.136	0.5	<100	35	7	0.2178	6.54E+04	0.8154

Table S4. Parameters of the Adams-Bohart and Wolborska model using linear regression analysis for As(V) adsorption onto PC-Fe/C-B under different conditions.

C_0 mg/L	Q mL/min	Dosage m g	Particle size mesh	T ℃	pH	Height of the column Z cm	Flow rate U_0 cm/min	Mass transfer coefficient k_{AB} L/mg·min	N_o mg/L	β_a min^{-1}	R^2
10	5.136	0.5	<100	35	3	1.23	10.22	0.004720	12.65	0.0597	0.9687
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
30	5.136	0.5	<100	35	3	1.23	10.22	0.002113	20.58	0.0435	0.8374
20	4.28	0.5	<100	35	3	1.23	8.51	0.002435	19.02	0.0463	0.9346
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
20	6.849	0.5	<100	35	3	1.23	13.63	0.002995	21.34	0.0639	0.8891
20	8.561	0.5	<100	35	3	1.23	17.03	0.003005	22.19	0.0667	0.7773
20	5.136	0.3	<100	35	3	0.74	10.22	0.004305	18.14	0.0781	0.8666
20	5.136	0.4	<100	35	3	0.98	10.22	0.003475	19.94	0.0693	0.9472
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
20	5.136	0.6	<100	35	3	1.48	10.22	0.002365	19.19	0.0454	6.5537
20	5.136	0.5	60-80	35	3	1.35	10.22	0.004880	8.86	0.0433	0.9308
20	5.136	0.5	80-100	35	3	1.29	10.22	0.002875	14.47	0.0416	0.8749
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
20	5.136	0.5	<100	25	3	1.23	10.22	0.003035	17.45	0.0530	0.9199
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
20	5.136	0.5	<100	45	3	1.23	10.22	0.002860	18.87	0.0540	0.9591
20	5.136	0.5	<100	35	**1**	1.23	10.22	0.002480	18.35	0.0455	0.8964
20	5.136	0.5	<100	35	2	1.23	10.22	0.002760	18.47	0.0510	0.9273
20	**5.136**	**0.5**	**<100**	**35**	**3**	**1.23**	**10.22**	**0.002865**	**18.52**	**0.0531**	**0.9307**
20	5.136	0.5	<100	35	4	1.23	10.22	0.002955	16.77	0.0496	0.9176
20	5.136	0.5	<100	35	5	1.23	10.22	0.003285	14.82	0.0487	0.8044
20	5.136	0.5	<100	35	6	1.23	10.22	0.002970	13.55	0.0402	0.8346
20	5.136	0.5	<100	35	7	1.23	10.22	0.002660	9.16	0.0244	0.9331

Table S5. Comparison of the adsorption capacity of the PC-Fe/C-B and various adsorbents for As(V) removal from water.

Sorbent	pH	Initial As(V) concentration (mg/L)	Surface area (m^2/g)	Grain size	T (°C)	Capacity (mg/g)	Ref.
PC-Fe/C-B	3	20	186.66	< 0.149 mm	35	12.37–21	This study
Iron-coated seaweeds	7	25			20	7.3	[1]
Biochar-magnetite composite	7	10	320.1	300–500 μm	25	5.49	[2]
Organo-modified natural zeolitic materials	7	10–500				6.7	[3]
Fe-sericite composite beads		50	13.51			5.78	[4]
Red mud-modified biochar (RM-BC)	6	10	186.95			5.923	[5]
PBGC-Fe/C	3	50	59.2	< 0.149 mm	35	4.83	[6]
Aluminum Mining By-product (AMB)	5.5–6.5	50		1 mm		4.51	[7]
CCHA nanocomposite	7	1–50			45	12.72	[8]
Zeo-NaY-S	6	20	506.6	21.70 μm		2.8	[9]
Bismuth impregnated biochar (BiBC500)	9.3	50	190.4	0.5–1 μm		16.21	[10]
Magnetic nanocomposite (FeeMWCNTs)		10		60–100 nm		250	[11]
Mesoporous sulphated zirconia (MSZ)	6.6	44.7	141			99.23	[12]
Potassium ferrate	6.5	2	250–600	1.5–3.0 nm		162.02	[13]
Mixed oxide (MO)	8	50	198 ± 2			20.7–12.9	[14]
Modified red mud	6.8	50	68.5		25	43.25	[15]
Zr(IV)-loaded SOW gel	3	15		75–150 μm	30	36.27	[16]
Synthetic zeolites H90	3.2	100	400			34.8	[17]
Polystyrene-Fe_3O_4	6	13				139.3	[18]
Magnetite nanoparticles	8	0.1	60	19.3 nm		0.485	[19]
Hematite nanoparticles	7.8	0.2	50			4.122	[20]
Fe_3O_4/RGO/Cu-ZEA		0.1	61.55			50	[21]
Mg–Fe-based hydrotalcites (FeHT)	9	2	1.448		25	0.103	[22]
Iron oxide amended rice husk char 950 IOA-RHC	6.85	0.1–2.5	308			1.46 ± 0.11	[23]
Fe(III)-modified montmorillonite	6	0.4	20.7		25	3.9	[24]

goethite-P(AAm) composite	7.2–7.7	0.3	5		25	1.22	[25]
Fe_3O_4@CTAB	6	1		10 nm		23.07	[26]
Chinese red soil	6	0.15	50.4		25	0.936	[27]
Carbonized yeast cells containing silver nanoparticles		2.5		19. 9 nm		1.14	[28]
Magnetic nanoparticles synthesized from waste red mud	2	0.05		6–14 nm	25	0.4	[29]
3D graphene macroscopic gel	4	0.93	13.22		30	0.24	[30]
Blast-furnace-slag geopolymer (BFS-GP)	7–8	2.4	64.5	5.93 μm		0.52	[31]
Aluminum modified crop straw-derived biochars	5	0.02–0.09	1.0–19.3		25	34.7–52.0	[32]
Bagasse fly ash	7	0.05	450	100–250 μm	25	0.0155	[33]
Granular TiO_2	8.2	0.8	196	0.18~0.25 mm		38.3	[34]
Iron oxide-based adsorbent μGFH	8	0.38	283 ± 3	< 5 μm	20 ± 2	22.4	[35]
Iron oxide-based adsorbent μTMF	8	0.38	178 ± 8	< 5 μm	20 ± 2	15.4	[35]

Table S6. Input files for the As(V) aqueous phase speciation in the simulation using PHREEQC.

```
SOLUTION_SPECIES        #As(V) speciation - log_k from phreeqc.dat
        H3AsO4 = AsO4-3 + 3H+
                log_k   -20.7
        H+ + AsO4-3 = HAsO4-2
                log_k   11.50
        2H+ + AsO4-3 = H2AsO4-
                log_k   18.46
```

Table S7. PHREEQC input files for the surface acid-base behavior of PC-Fe/C-B in aqueous As(V) solution.

```
SURFACE_MASTER_SPECIES
    Surf_iron          Surf_ironOH
SURFACE_SPECIES
        # Dixit and Hering. Environ Sci Technol 37 (2003) 4182 [36]
    Surf_ironOH = Surf_ironOH
                            log_k       0
    Surf_ironOH = Surf_ironO- + H+
                            log_k       -8.93
    Surf_ironOH + H+ = Surf_ironOH2+
                            log_k       7.29
        # Stachowicz et al. J Colloid & Interface Sci 302(2006)62 [37]
    2Surf_ironOH + 2H+ + AsO4-3 = Surf_iron2O2AsO2-1 + 2H2O
                            log_k       29.29
    2Surf_ironOH + 3H+ + AsO4-3 = Surf_iron2O2AsOOH + 2H2O
                            log_k       32.69
    1Surf_ironOH + 2H+ + AsO4-3 = Surf_ironOAsO2OH-1 + H2O
                            log_k       26.62
```

Table S8. An input file example of the CD-MUSIC model for surface complexation in the simulation using PHREEQC.

```
SURFACE 1 CD_MUSIC surface with Donnan layer
    -equilibrate with solution 1
    -sites_units   density
    -cd_music
    Surf_ironOH      2.50 186.66      0.50
            # Name of a surface binding site
            # Total number of surface binding site (site/nm2)
            # Surface area (m2/g)
            # Mass of adsorbent (g)
    -capacitances      0.85 0.75
            # c1—Capacitance for the 0-1 plane in the CD-MUSIC formulation, F/m2.
        Stachowicz (2006) [37]
            # c2—Capacitance for the 1-2 plane in the CD-MUSIC formulation, F/m2.
        Hiemstra(2006) [38]
    -Donnan      1e-8
            # Thickness of the diffuse layer in meters. Default is 10-8 m.
    -only_counter_ions       true
            # True indicates that the surface charge will be balanced
            # by a surplus of counter-ions in the diffuse layer.
```

Table S9. An input file example for the influent TRANSPORT in the simulation using PHREEQC.

```
TRANSPORT
    -cells 10                 #Number of cells in a 1D column with 0.5 g adsorbent
    -lengths 0.00123          #Length (m) of each cell with 0.05 g adsorbent
    -time_step 2.54           #Time (s) of each shift for Q = 5.136 mL/min
    -shifts 11000             #Number of shifts periods in simulation
    -flow_direction forward
    -boundary_conditions flux flux
    -diffusion_coefficient 0
    -dispersivities 0.02
    -correct_disp true
    -punch_cells 10
    -punch_frequency 1
    -print_cells 10
    -print_frequency 20
```

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