Electronic Supplementary Material (ESI) for RSC Advances.

Batch and Continuous Packed-Bed Column Sorption of Metal Ions using Economically Derived Ca-MOF Immobilized Cellulose Porous Matrix

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Supplementary file

Table S1 Different isotherms and kinetic models were used to fit the sorption equilibrium and kinetic data.

	Non-linear Equations	Model parameters	Other variables
Isotherm models			
Langmuir	$\theta = \frac{q_e}{q_m} = \frac{bC_e}{1 + bC_e}$ Sub Eq. $R_L = \frac{1}{1 + bC_0}$	q_m, monolayer sorption capacity mg g^{-1}. b, affinity of union sites.	θ, fractional coverage. C_e, equilibrium concentration of solute in the solution mg L^{-1}. q_e, equilibrium sorption capacity mg g^{-1}. R_L, is a separation factor C_o, maximum concentration at equilibrium.
Freundlich	$q_e = K_f C_e^{\frac{1}{n}}$	K_f, sorption capacity related to bond energy (mg g^{-1}) (L mg^{-1})$^{1/n}$. n, sorption intensity.	q_e, equilibrium adsorption capacity mg g^{-1}. C_e, equilibrium concentration mg L^{-1}.
Temkin	$q_e = \frac{RT}{b_T} \ln (A_T C_e)$ Sub Eq. $B = RT/b_T$	A_T, equilibrium binding constant. b_T, Temkin constant.	T, absolute temperature K. R, universal gas constant, 8.314 J mol^{-1} K^{-1}. B, constant related to heat of adsorption J mol^{-1}.
D-R	$q_e = q_m \exp(-K\varepsilon^2)$ Where;	K, D-R constant mol^{-2} K^{-1} J^{-2}. q_m, monolayer sorption capacity mg g^{-1}.	C_e, equilibrium concentration mg L^{-1}. T, absolute temperature K. R, universal gas constant, 8.314 J mol^{-1} K^{-1}.

	$\varepsilon = RT * \ln\left(1 + \frac{1}{C_e}\right)$ Sub Eq. $E = \frac{1}{(2K)^{\frac{1}{2}}}$		*E,* mean free energy kJ mol^{-1}.
Kinetic models			
Pseudo-first order	$q_t = q_e\left(1 - e^{k_1 t}\right)$	q_e, equilibrium sorption capacity mg g^{-1}. k_1, pseudo-first-order rate constant min^{-1}.	q_t, sorption capacity at time 't' mg g^{-1}.
Pseudo- second-order	$q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t}$	q_e, equilibrium sorption capacity mg g^{-1}. k_2, pseudo-second-order rate constant g mg^{-1}min^{-1}.	q_t, sorption capacity at time 't' mg g^{-1}.

Table S2 Predicted breakthrough points from the constants of the BDST model for different influent concentrations (Q: 5 mL min^{-1}, Z: 20 cm).

			300 mg L^{-1}				
C_t/C_0	a (min cm^{-1})	b (min)	a' (min cm^{-1})	b' (min)	$t_{pred.}$ (min)	$t_{exp.}$ (min)	E (%)
0.01	31	300	51.66	118.51	914.81	530	72.60
0.1	38	300	63.33	145.28	1121.38	1440	-22.12
0.5	60	270	100.00	229.39	1770.61	2400	-26.22
0.9	69	200	115.00	263.79	2036.20	3140	-35.15

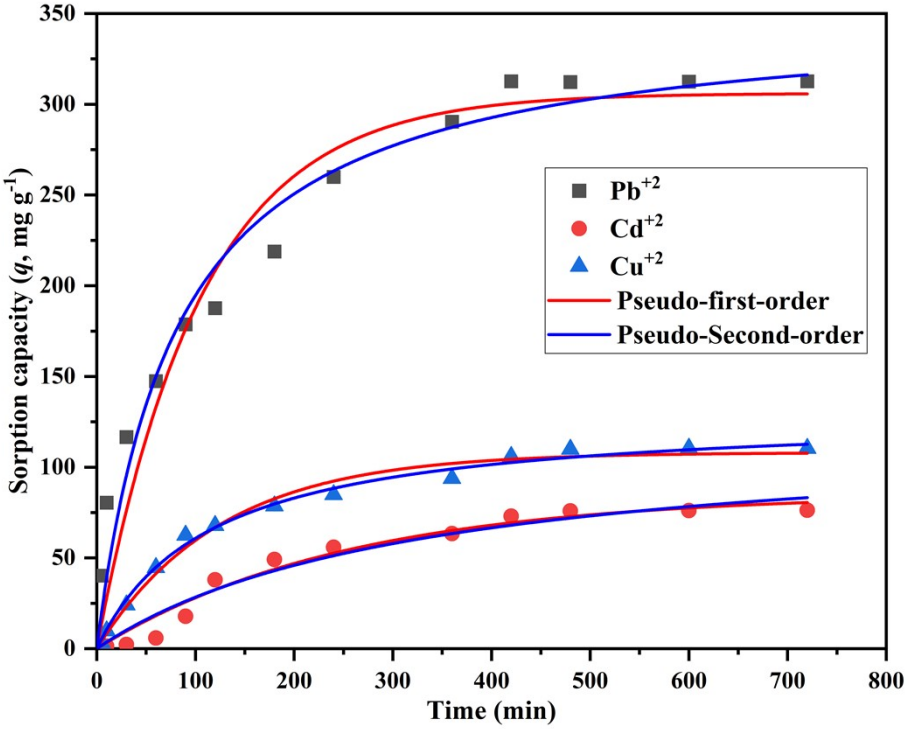

Fig. S1 Applicability of kinetic models for the sorption of (a) Pb^{+2}, (b) Cd^{+2}, and (c) Cu^{+2} ions using Ca-MOF-CB.

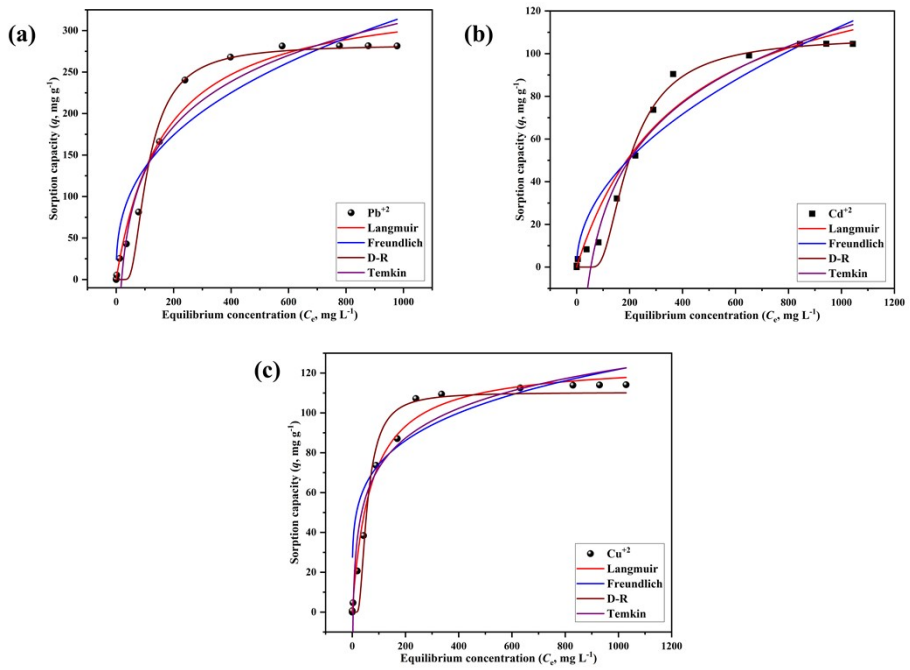

Fig. S2 Applicability of isotherm models for the sorption of (a) Pb^{+2}, (b) Cd^{+2}, and (c) Cu^{+2} ions using Ca-MOF-CB.

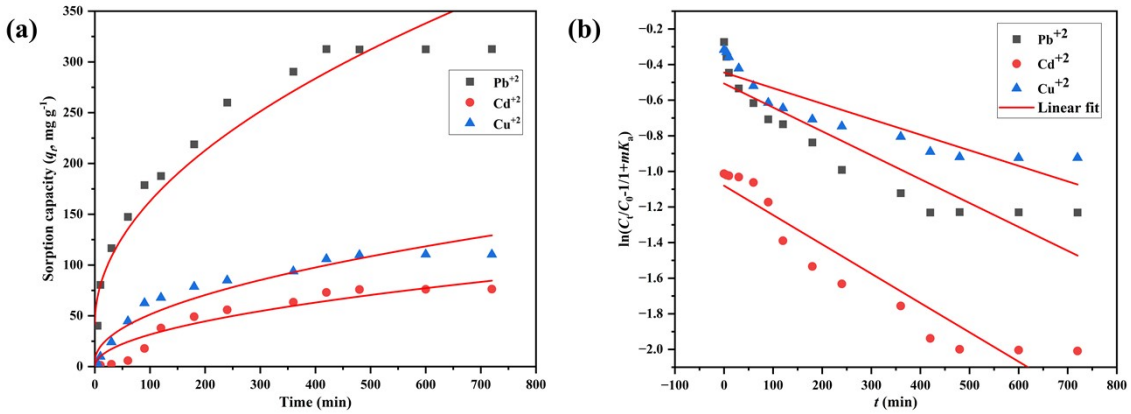

Fig. S3 Plots determining kinetic parameters of (a) intra-particle diffusion and (b) external film diffusion.

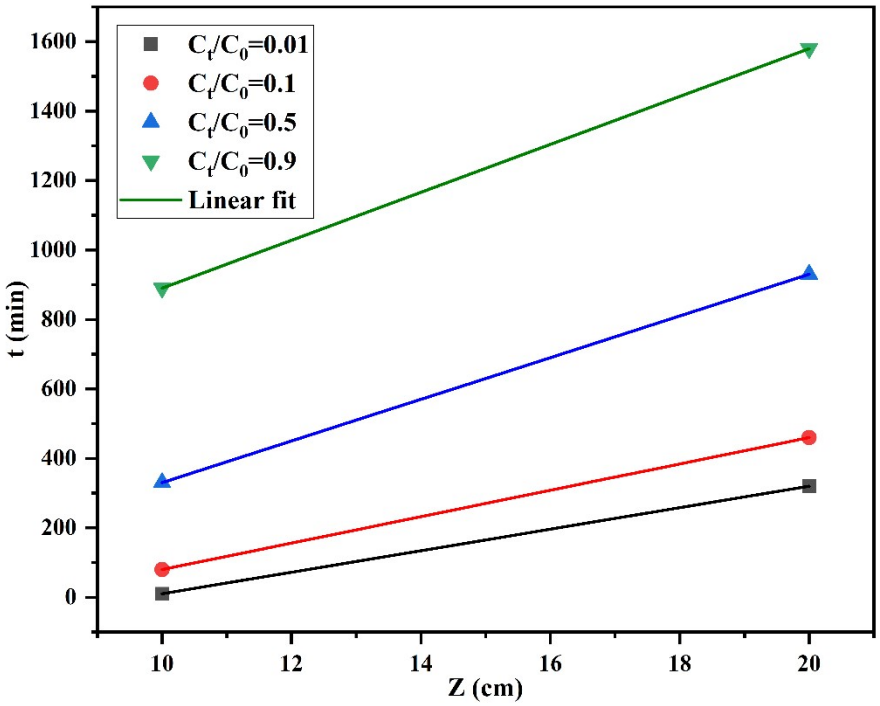

Fig. S4 Applicability of the BDST model to the experimental run.