Systematic evaluation for the impact of the geological conditions on the adsorption affinities of calcite as an adsorbent of Zn^{2+} ions from aqueous solutions: experimental and theoretical studies

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Table.S1. Nonlinear equations of kinetic, classic isotherm, and advanced isotherm models

Kinetic models		
Model	**Equation**	**Parameters**
Pseudo-first-order	$q_t = q_e (1 - e^{-k_1.t})$	q_t (mg/g) is the adsorbed ions at time (t), and K_1 is the rate constant of the first-order adsorption (min^{-1})
Pseudo-second-order	$q_t = \dfrac{q_e^2 k_2 t}{1 + q_e k_2 t}$	q_e is the quantity of adsorbed ions after equilibration (mg/g), and K_2 is the model rate constant (g/mg min).
Intra-particle diffusion	$q_t = kt^{0.5} + C$	k_p (mg g^{-1} min$^{-0.5}$) is the intraparticle diffusion rate constant and C is the intercept of the line

Classic Isotherm models		
Model	**Equation**	**Parameters**
Langmuir	$Q_e = \dfrac{Q_{max}\, bC_e}{(1 + bC_e)}$	C_e is the rest ions concentrations (mg/L), Q_{max} is the theoritical maximum adsorption capacity (mg/g), and b is the Langmuir constant (L/mg)
Freundlich	$Q_e = K_f C_e^{1/n}$	K_F (mg/g) is the constant of Freundlich model related to the adsorption capacity and n is the constant of Freundlich model related to the adsorption intensities
Dubinin–Radushkevich	$Q_e = Q_m e^{-\beta \varepsilon^2}$	β (mol^2/KJ^2) is the D-R constant, ε (KJ^2/mol^2) is the polanyil potential, and Q_m is the adsorption capacity (mg/g)

Advanced isotherm models		
Model	**Equation**	**Parameters**
Monolayer model with one energy site (Model 1)	$Q = nN_o = \dfrac{nN_M}{1 + (\frac{C1/2}{C})^n} = \dfrac{Q_o}{1 + (\frac{C1/2}{C})^n}$	Q is the adsorbed quantities in mg/g

n is the number of adsorbed ion per site |
| **Monolayer model with two energy sites (Model 2)** | $Q = \dfrac{n_1 N_{1M}}{1 + (\frac{C_1}{C})^{n_1}} + \dfrac{n_2 N_{2M}}{1 + (\frac{C_2}{C})^{n_2}}$ | Nm is the density of the effective receptor sites (mg/g)

Q_o is the adsorption capacity at the saturation state in mg/g |
| **Double layer model with one energy site (Model 3)** | $Q = Q_o \dfrac{(\frac{C}{C1/2})^n + 2(\frac{C}{C1/2})^{2n}}{1 + (\frac{C}{C1/2})^n + (\frac{C}{C1/2})^{2n}}$ | C1/2 is the concentration of the ions at half saturation stage in mg/L

C1 and C2 are the concentrations of the ions at the half saturation stage for the first active sites and the second active sites, respectively |
| **Double layer model with two energy sites (Model 3)** | $Q = Q_o \dfrac{(\frac{C}{C1})^n + 2(\frac{C}{C2})^{2n}}{1 + (\frac{C}{C1})^n + (\frac{C}{C2})^{2n}}$ | n1 and n2 are the adsorbed ions per site for the first active sites and the second active sites, respectively |