

Insight into the wheat residues-derived adsorbents for the remediation of organic and inorganic aquatic contaminants: A review

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Supplementary Data

Table S1. The names and forms of common adsorption models and error functions.

Table S1

Relation	Formula	Parameters definition	Ref.
Isotherm model			
Langmuir	$q_e = \frac{q_L K_L C_e}{1 + K_L C_e}$ $R_L = \frac{1}{1 + K_L C_o}$	q_e (mg/g): Equilibrium adsorbed amount C_e (mg/L) : Equilibrium residual amount q_L (mg/g): Langmuir predicted adsorbed amount K_L (L/mg): Langmuir affinity parameter R_L : Favorability parameter C_o (mg/L): Maximum inlet amount	(Langmuir, 1916)
Freundlich	$q_e = K_F C_e^{1/n}$	K_F ((mg/g) (L/mg) ^{1/n}): Adsorbed amount parameter $1/n$: Adsorption intensity parameter	(Freundlich, 1906)
Temkin	$q_e = B_T \ln K_T C_e$	B_T : Temkin constant related to adsorption heat K_T (L/mg): Equilibrium binding constant	(Temkin & Pyzhev, 1940)
Dubinin–Radushkevich	$q_e = q_D e^{\left\{-K_D (RT \ln(1 + \frac{1}{C_e}))^2\right\}}$	q_D (mg/g): D–R predicted adsorbed amount K_D : D–R constant.	(Dubinin & Radushkevich, 1947)
Sips	$q_e = \frac{q_s K_s C_e^{1/m}}{1 + K_s C_e^{1/m}}$	q_s (mg/g) : Sips predicted adsorbed amount K_s (L/mg) ^{1/m} : Sips affinity parameter $1/m$: Heterogeneity index	(Sips, 1948)
Kinetic model			
Pseudo-first Order (PFO)	$q_t = q_e (1 - e^{-k_1 t})$	q_t (mg/g): Instant adsorbed amount k_1 (1/min): Apparent PFO rate constant	(Lagergren, 1898)
Pseudo-second Order (PSO)	$q_t = \frac{k_2 q_e^2 t}{1 + k_2 q_e t}$	k_2 (g/mg.min): Apparent PSO rate constant	(Ho & McKay, 1999)

Intraparticle diffusion	$q_t = k_{di} t^{1/2} + C_i$	k_{di} (mg/g.min ^{1/2}): Rate constant C_i (mg/g): Adsorption degree parameter	(Weber & Morris, 1963)
Elovich	$q_t = \frac{1}{\beta} \ln(1 + \alpha \beta t)$	α (mg/g min): Primary rate of adsorption β : Desorption parameter	(Roginsky & Zeldovich, 1934)
Thermodynamic models			
Van't Hoff	$\ln(K_d) = \frac{\Delta S^\circ}{R} - \frac{\Delta H^\circ}{RT}$	K_d : Distribution coefficient for the adsorption. ΔS° (J/mol.K): Change in entropy ΔH° (J/mol): Change in enthalpy	(Sari & Tuzen, 2008)
Gibbs	$\Delta G^\circ = -RT \ln(K_d)$	R (J/mol.K): Universal gas constant (8.314) T (K): temperature ΔG° (J/mol): Change in free energy	(Sari et al., 2008)
Error function			
Coefficient of Determination (R^2)	$R^2 = 1 - \frac{\sum_{i=1}^n (q_{e, \text{exp}} - q_{e, \text{cal}})^2}{\sum_{i=1}^n (q_{e, \text{exp}})^2 - [(\sum_{i=1}^n q_{e, \text{exp}})^2 / n]}$	n : Number of applied data q_{exp} and q_{cal} (mg/g): Observed and predicted adsorbed amounts	(Boulinguez et al., 2008)
Chi- square statics (χ^2)	$\chi^2 = \sum_{i=1}^n \frac{(q_{e, \text{exp}} - q_{e, \text{cal}})^2}{q_{e, \text{cal}}}$	n : Number of applied data q_{exp} and q_{cal} (mg/g): Observed and predicted adsorbed amounts	(Boulinguez et al., 2008)

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