

Supporting Information

Levofloxacin adsorption onto MWCNTs/CoFe₂O₄ nanocomposites: Mechanism, and modelling using non-linear kinetics and isotherm equations

Tariq J. Al-Musawi¹, Ethar M. Al-Essa², Nezamaddin Mengelizadeh³, Fatemeh Ganji⁴, Davoud Balarak^{5,*}

¹Building and Construction Techniques Engineering Department, Al-Mustaqbal University College, 51001 Hillah, Babylon, Iraq.

²Department of Civil Engineering, Isra University, Amman, Jordan.

³Department of Environmental Health Engineering, Evas Faculty of Health, Larestan University of Medical Sciences, Larestan, Iran.

⁴Student Research Committee, Zahedan University of Medical Sciences, Zahedan, Iran.

⁵Department of Environmental Health, Health Promotion Research Center, Zahedan University of Medical Sciences, Zahedan, Iran.

***Corresponding author:**

Prof. Dr. Davoud Balarak

Email: dbalarak2@gmail.com.

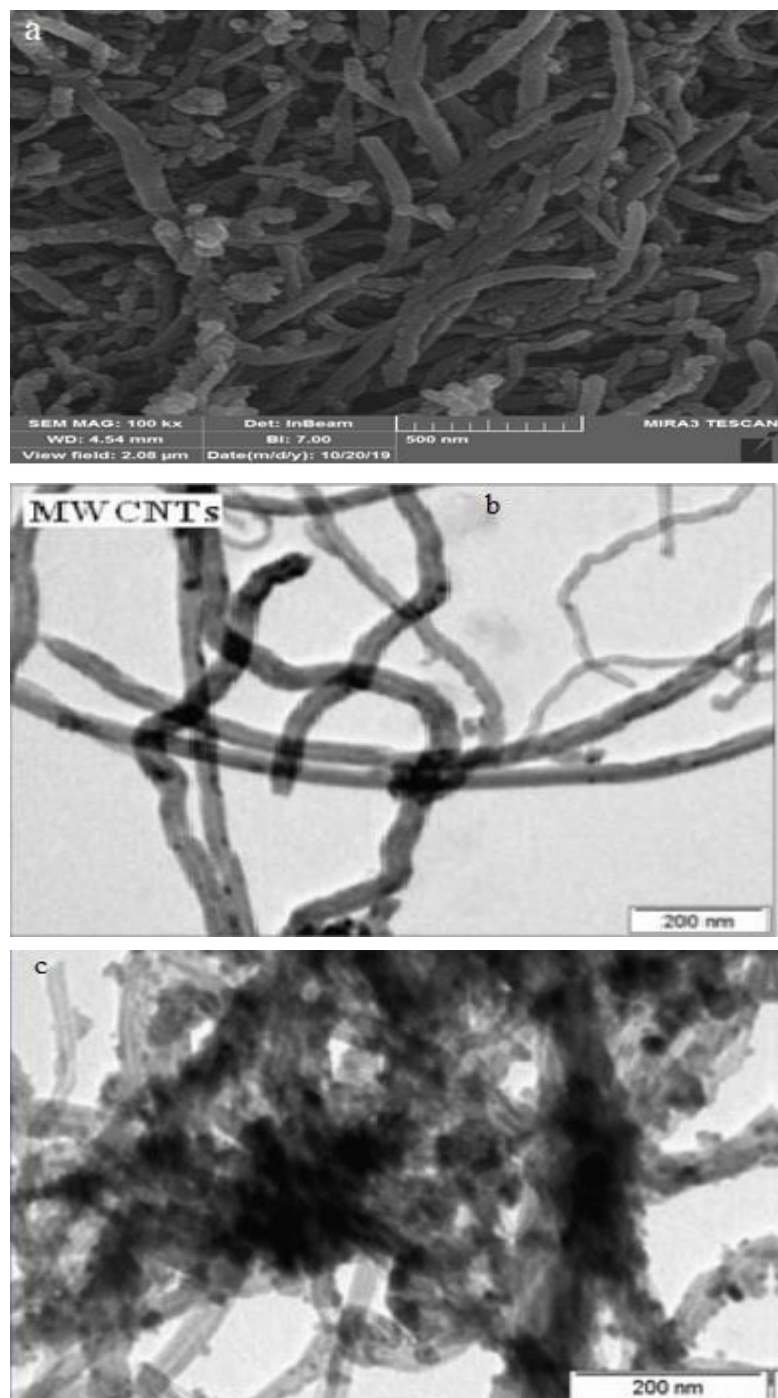


Figure S1. SEM image of MWCNTs/CoFe₂O₄ (a), TEM image of MWCNTs (b), and TEM image of MWCNTs/CoFe₂O₄ (c)

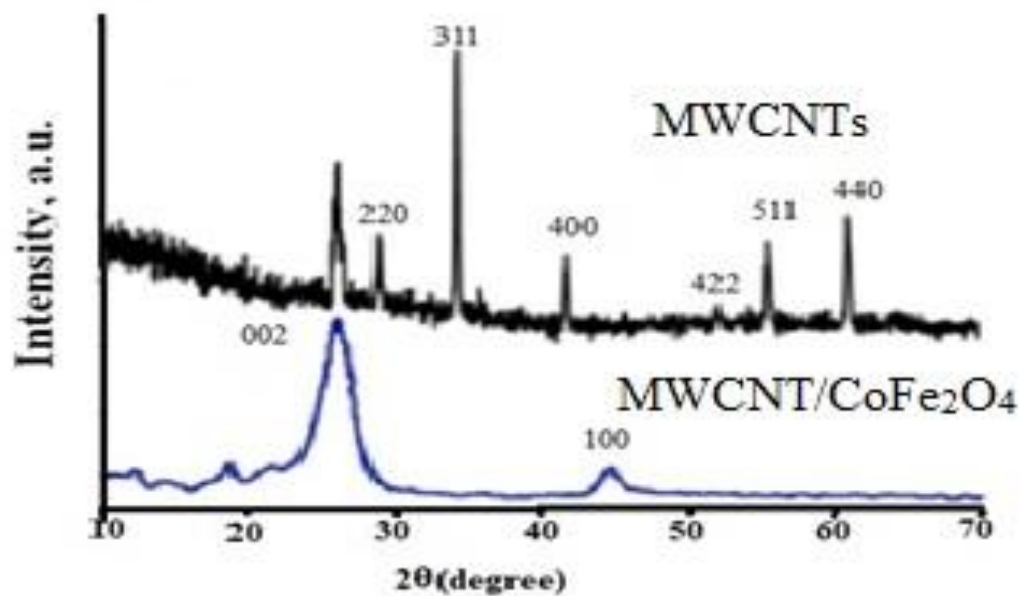


Figure S2. XRD patterns of the MWCNTs and MWCNTs/CoFe₂O₄

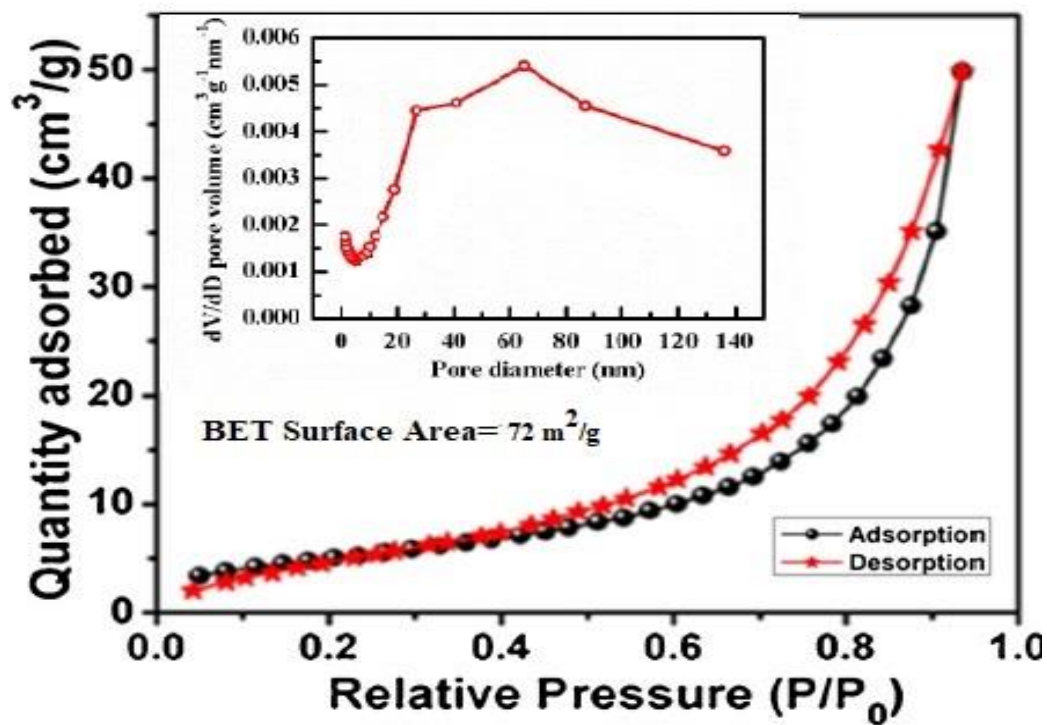


Figure S3. N₂ adsorption-desorption isotherms and pore size distribution

Table S1: Errors functions used to determine the goodness of fit of the experimental data with relevant theoretical model

Error function	Abbreviation	Formula	References
Residual Root Mean Square Error	RMSE	$\sqrt{\left(\frac{1}{n-1} \sum_{i=1}^n (q_{e,exp} - q_{e,cal})\right)^2}$	[1]
Average Relative Error	ARE	$\frac{100}{n} \sum_{i=1}^n \left \frac{q_{e,exp} - q_{e,cal}}{q_{e,exp}} \right _i$	[2]
Sun of absolute errors	EABS	$\sum_{i=1}^n q_{e,exp,i} - q_{e,cal,i} $	[3]
Hybrid fractional error function	HYBRID	$\frac{100}{n-p} \sum_{i=1}^n \left[\frac{(q_{e,exp} - q_{e,cal})^2}{q_{e,exp}} \right]$	[4]
Nonlinear chi-square test	χ^2	$\sum_{i=1}^n \frac{(q_{e,cal} - q_{e,exp})^2}{q_{e,exp}}$	[5]
Coefficient of determination	R^2	$\frac{(q_{e,exp} - \overline{q_{e,cal}})^2}{\sum (q_{e,exp} - \overline{q_{e,cal}})^2 + (q_{e,exp} - q_{e,cal})^2}$	[4]

Table S2: Non-linear forms of kinetic models

Kinetic	Equation	References
Pseudo-first-order kinetic model (PFO)	$q_t = q_e(1 - e^{-k_1 t})$ K_1 : Equilibrium rate constant for pseudo-first order kinetics (1/min)	[6]
Pseudo-second-order kinetic model (PSO)	$q_t = \frac{k_2 q_e^2 t}{1 + k_2 q_e t}$ K_2 : Equilibrium rate constant for pseudo-second order kinetics (PSO) (g/mg. min)	[7]
Elovich	$q_t = \frac{\ln(\alpha\beta)}{\beta} + \frac{\ln(t)}{\beta}$ α : Indicates the chemical adsorption rate (mg/mg min), β : Coefficient in relation to the extension of covered surface and activation energy of chemical adsorption (g/mg).	[8]
Intraparticle diffusion kinetic model (IPD)	$q_t = K_{id} t^{1/2} + C$ K_b : Intra-particle Diffusion (IPD) rate constant (mg/g. min ^{1/2}), C: Thickness of the boundary layer (mg/g)	[5]

Table S3: Non-linear forms of isotherms models

Isotherm	Equation	References
Langmuir	$Q_e = \frac{Q_m K_L C_e}{1 + K_L C_e}$ <p>K_L: Langmuir adsorption constant (l/mg), q_m: Maximum adsorption capacity (mg/g), R_L: Dimensionless separation factor, the values of R_L show whether the adsorption process is irreversible ($R_L = 0$), linear ($R_L = 1$), favorable ($0 < R_L < 1$) or undesirable ($R_L > 1$).</p>	[9]
Freundlich	$Q_e = K_F C_e^{1/n}$ <p>K_F: Freundlich constant (mg/g)(L/mg)^{1/n}, n: Heterogeneity factor. If the value of $n < 1$, the adsorption is a chemical process; if $n > 1$, then it is a physical process.</p>	[4]
Dubinin-Radushkevitch (D-R)	$Q_e = Q_m \exp(-K' \varepsilon^2), \varepsilon = RT \ln(1 + \frac{1}{C_e})$ $E = (2K_D)^{-1/2}$ <p>B: Activity coefficient constant (mol²/kJ²), ε: Polanyi potential (kJ/mol), which is equal to $RT \ln(1 + \frac{1}{C_e})$, where R is the ideal gas constant (8.314 J/(mol.K)), and T is the thermodynamic absolute temperature (K), E: The adsorption energy (kJ/mol), which is equal to $\frac{1}{\sqrt{-2\beta}}$.</p>	[10]
Temkin	$(q_e = B_T \ln(K_T C_e))$ <p>K_T: Constant of equilibrium binding (L/mg), B_T: Temkin constant associated with the heat of adsorption (J/mol).</p>	[11]
Redlich-Peterson	$q_e = \frac{A_{RP} C_e}{1 + B_{RP} C_e^{\beta_{RP}}}$ <p>A_{RP}: Redlich–Peterson isotherm constant (L/g)</p> <p>B_{RP}: Redlich–Peterson isotherm constant $(\frac{L}{mg})^{\beta_{RP}}$, β_{RP}: An exponent which lies between 0 and 1</p>	[8]
Sips	$q_e = \frac{K_s C_e^{\beta_s}}{1 + a_s C_e^{\beta_s}}$ <p>K_s: Sips model isotherm constant $(\frac{mg}{g})(\frac{L}{mg})^{\beta_s}$</p> <p>$a_s$: Sips model isotherm constant $(\frac{L}{mg})^{\beta_s}$, β_s: An exponent which lies between 0 and 1</p>	[12]
Toth	$(q_e = \frac{q_m K_T C_e}{(1 + (K_T C_e)^n)^{\frac{1}{n}}})$ <p>q_m: Maximum adsorption capacity (mg/g)</p> <p>K_T: Toth isotherm constant (L/mg)</p> <p>n: Toth isotherm constant ($0 < n \leq 1$)</p>	[13]

Hill	$(q_e = \frac{Q_{SH}C_e^{nH}}{K_D + C_e^{nH}})$ <p>Q_{SH}: saturation for maximum uptake (mg/L)</p> <p>K_D: Hill constant, nH: coefficient of binding interaction. $nH > 1$, positive cooperatively in binding, $nH = 1$, non-cooperative or hyperbolic binding, $nH < 1$, negative cooperatively in binding</p>	[3]
Kahn	$(Q_e = \frac{q_m b_K C_e}{(1 + b_K C_e)^{a_K}})$ <p>q_m: Maximum adsorption capacity (mg/g)</p> <p>b_K: Khan model constants, a_K: is the Khan model exponent</p>	[14]

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