

Supplementary Information

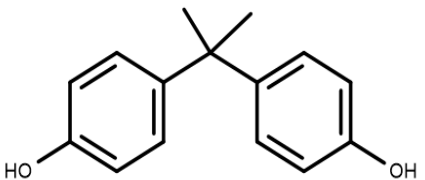
Magnetite Doped Metal-Organic Framework Nanocomposites: An Efficient Adsorbent for Removal of Bisphenol-A Pollutant

Okan Icten*, Demet Ozer

Hacettepe University, Faculty of Science, Department of Chemistry, Ankara, Turkey

[*okanicten@hacettepe.edu.tr](mailto:okanicten@hacettepe.edu.tr)

Table S1. The general physicochemical properties of BPA

| Properties | Bisphenol A |
|---------------------------|--|
| Structure |  |
| Usage | Plastic and resin |
| Formula | C ₁₅ H ₁₆ O ₂ |
| CAS number | 80-05-7 |
| MW (g/mol) | 228.29 |
| MV (cm ³ /mol) | 199.5 |
| pKa | 9.6 |
| LogK _{ow} | 3.32 |
| Diameter (Å) | 7.5 |
| Dipole moment (Debye) | 1.41 |

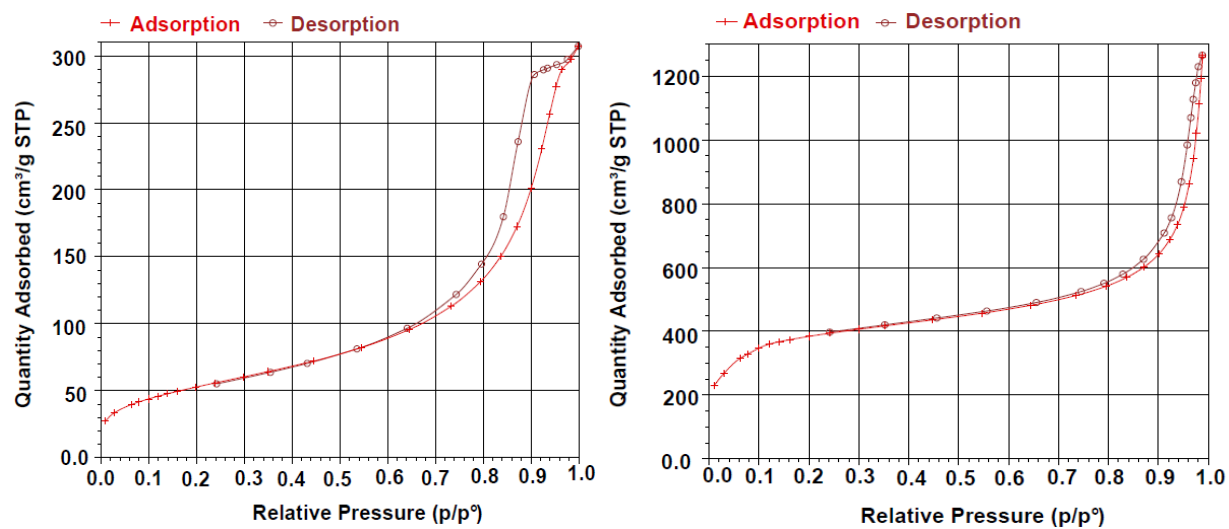


Fig. S1. N₂ adsorption/desorption isotherms of (a) Fe₃O₄@Dex, and (b) MOF:Fe₃O₄@Dex(80) nanocomposite structures.

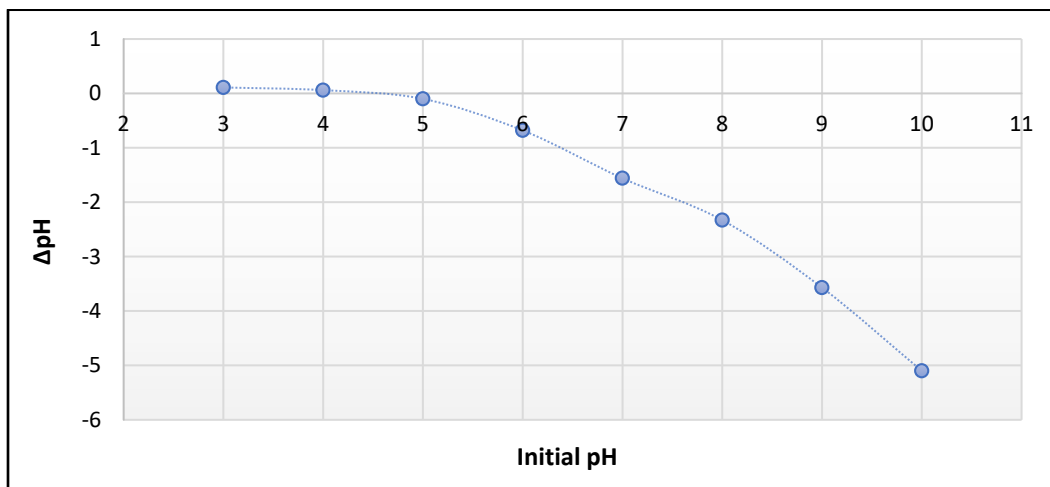


Fig. S2. Experimental immersion technique curves for MOF:Fe₃O₄@Dex nanocomposite

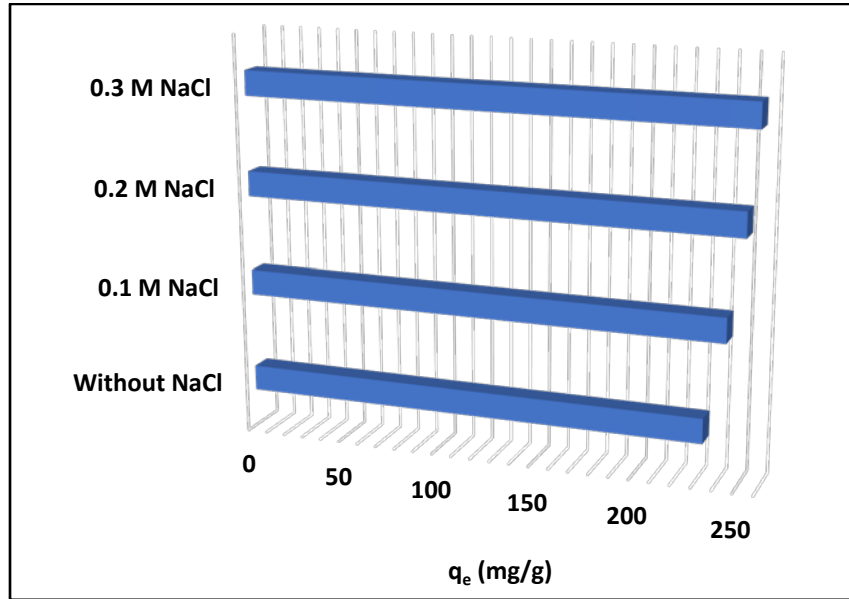


Fig. S3. Effects of NaCl concentrations

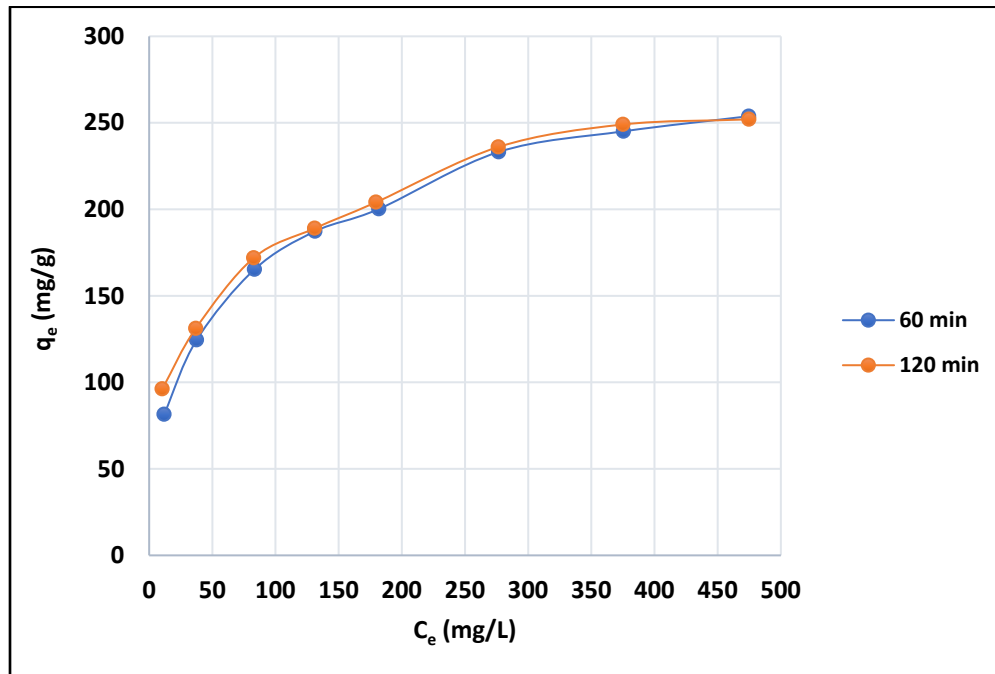


Fig. S4. Experimental isotherm curve

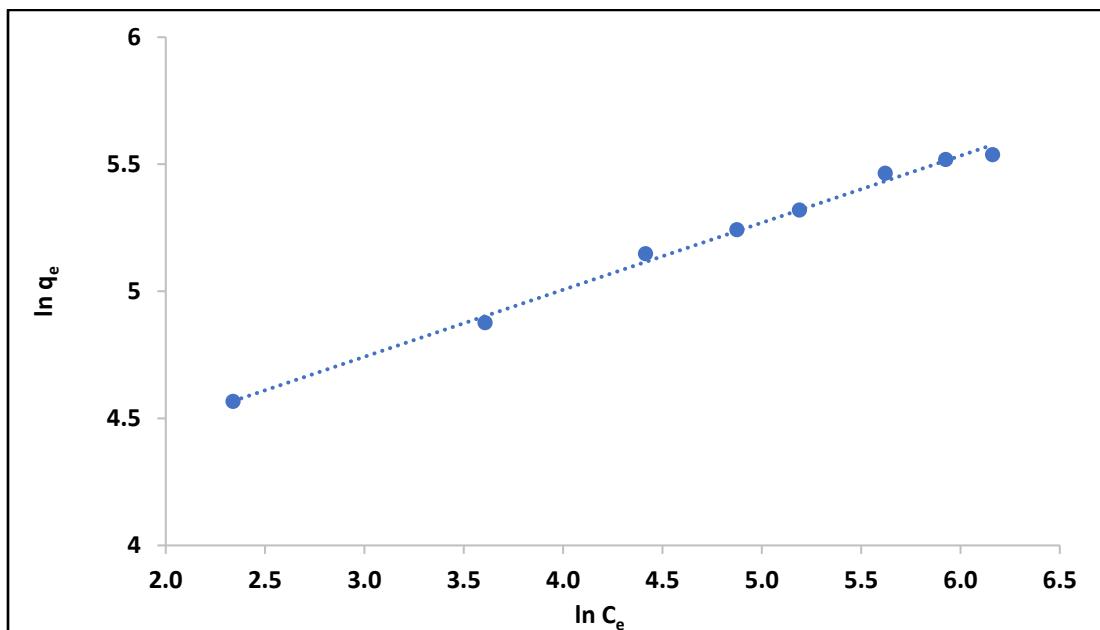


Fig. S5. Freundlich adsorption isotherm

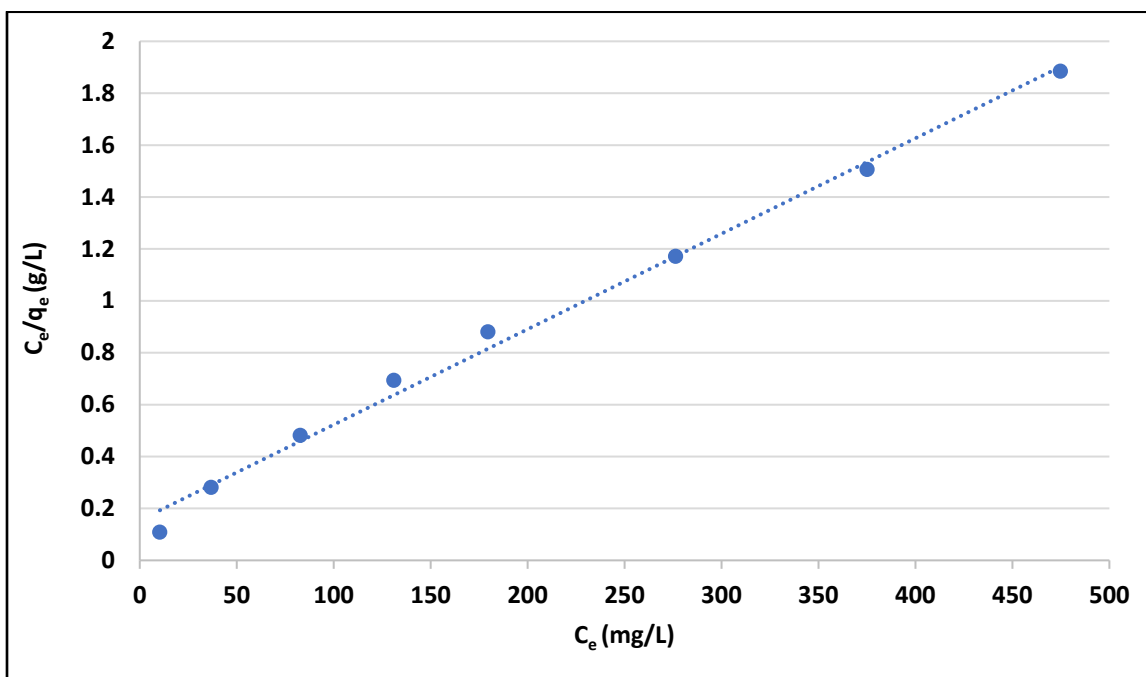


Fig. S6. Langmuir adsorption isotherm

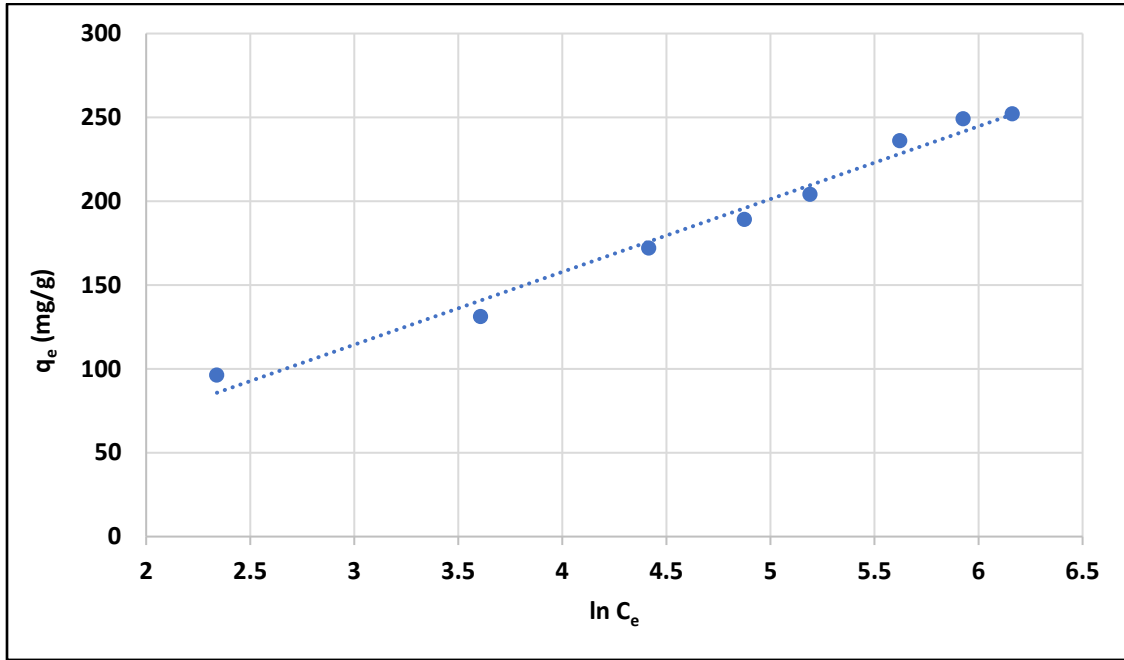


Fig. S7. Temkin adsorption isotherm

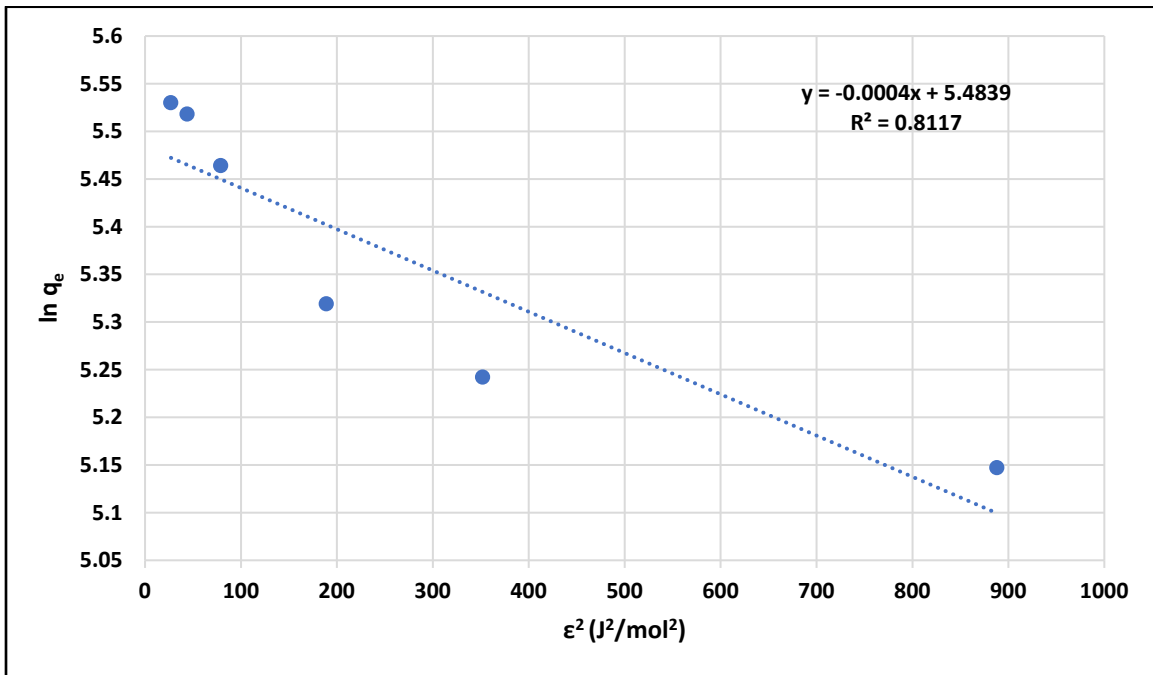


Fig. S8. Dubinin-Redushkevich isotherm (D-R model)

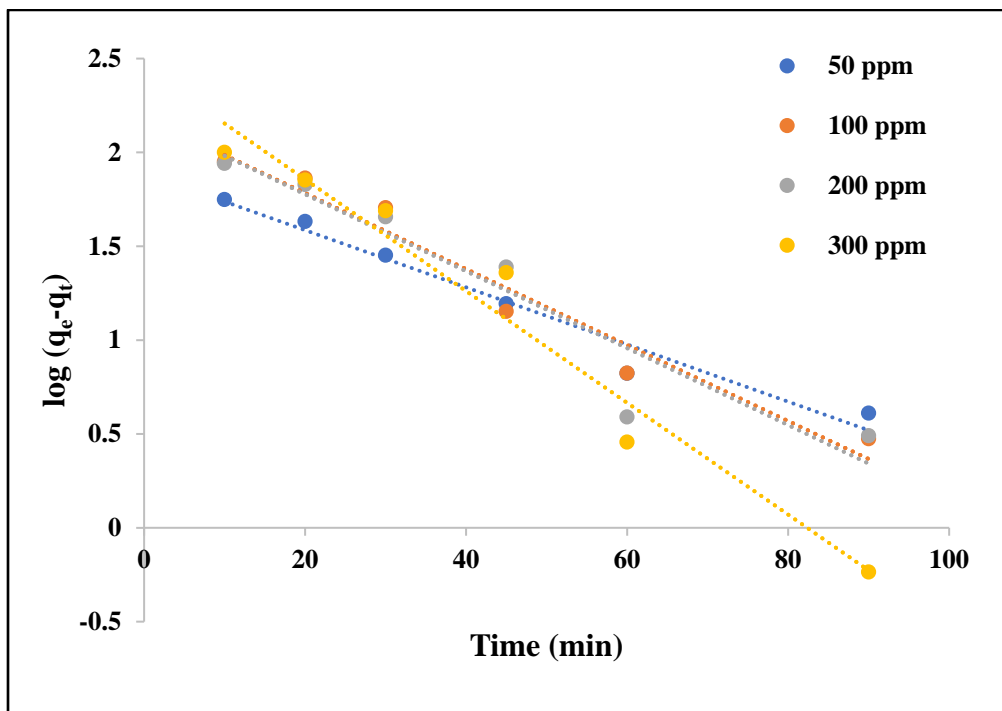


Fig. S9. Pseudo-first order kinetic plots for the adsorption of BPA using MOF:Fe₃O₄@Dex(80) composite at different initial BPA concentrations

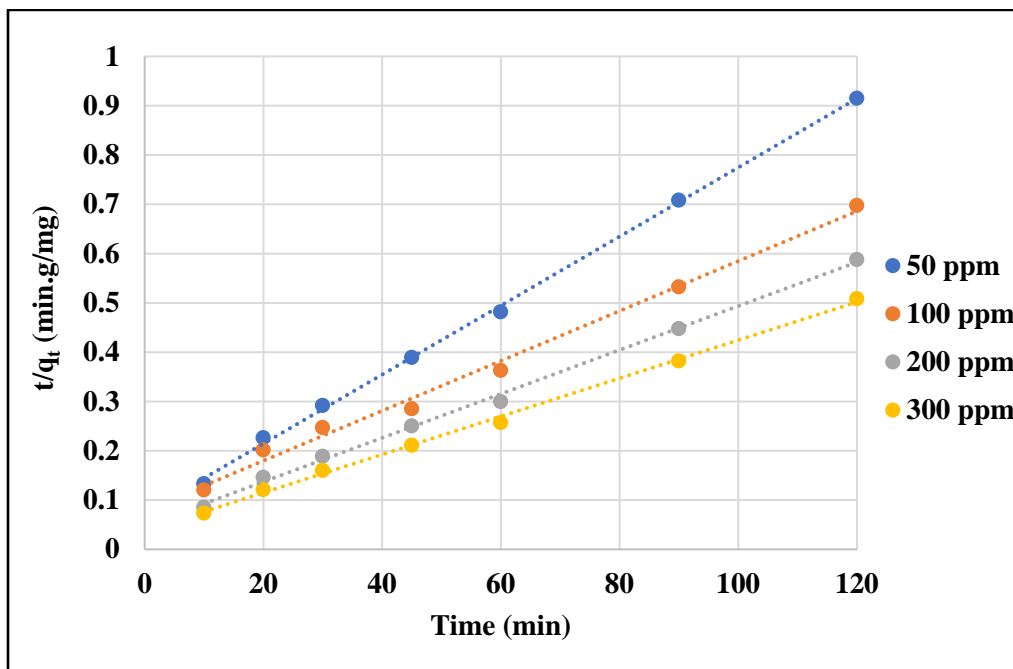


Fig. S10. Pseudo-second order kinetic plots for the adsorption of BPA using MOF:Fe₃O₄@Dex(80) composite at different initial BPA concentrations

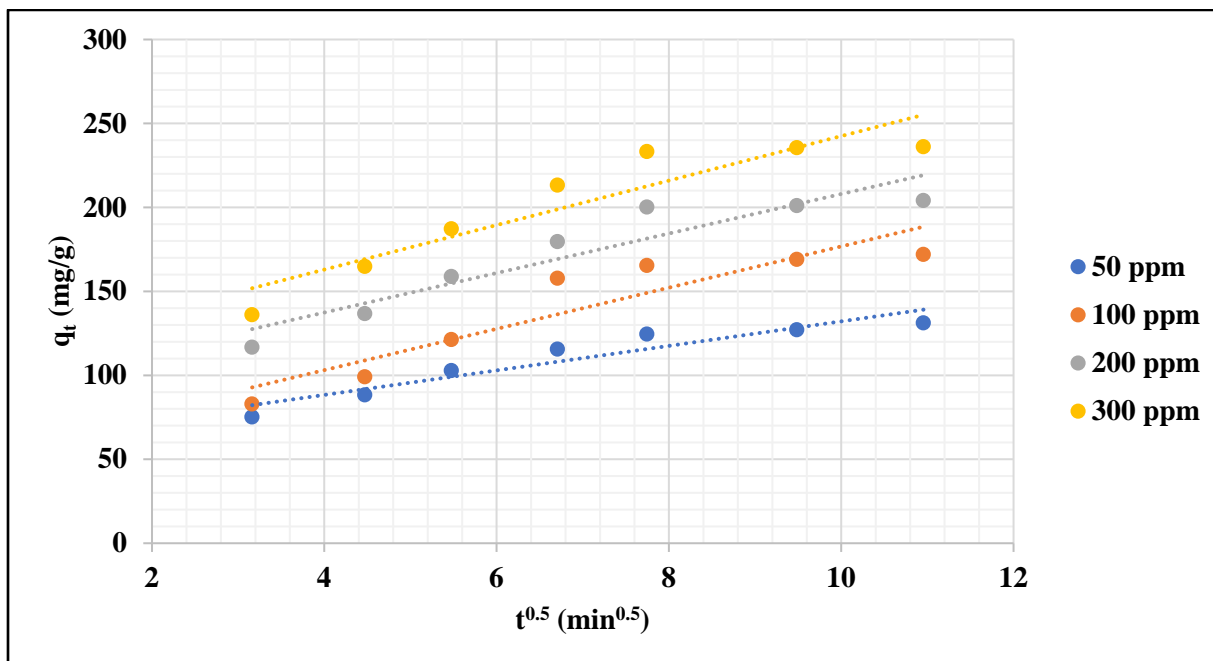


Fig. S11. The intraparticle diffusion model for the adsorption of BPA using MOF:Fe₃O₄@Dex(80) composite at different initial BPA concentrations

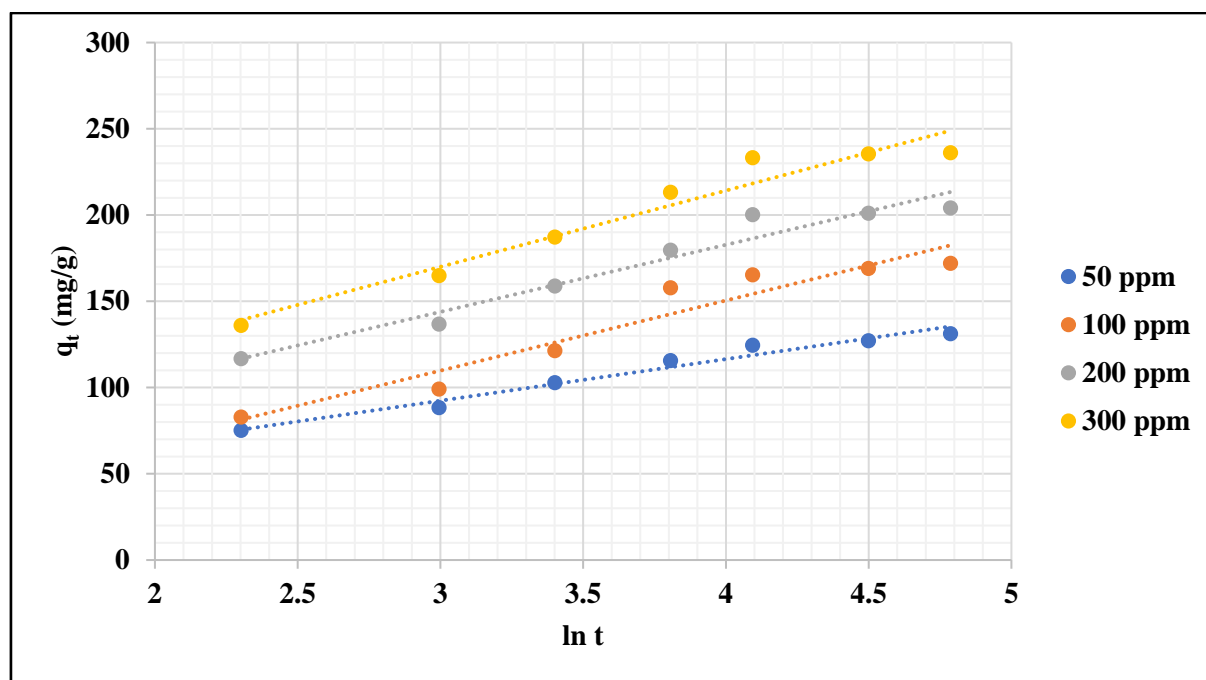


Fig. S12. The Elovich model for the adsorption of BPA using MOF:Fe₃O₄@Dex(80) composite at different initial BPA concentrations

ADSORPTION AND KINETIC EQUATIONS^{1,2}

$$\frac{C_e}{q_e} = \frac{1}{K_L q_m} + \frac{C_e}{q_m} \quad (\text{equation S1})$$

$$\ln q_e = \ln K + \frac{1}{n} \ln C_e \quad (\text{equation S2})$$

$$R_L = \frac{1}{1 + bC_i} \quad (\text{equation S3})$$

$$q_e = B \ln A + B \ln C_e \quad (\text{equation S4})$$

$$\ln q_e = \ln q_m - \beta \varepsilon^2 \quad (\text{equation S5})$$

$$\varepsilon = RT \ln \left(1 + \frac{1}{C_e} \right) \quad (\text{equation S6})$$

$$E = \frac{1}{\sqrt{2\beta}} \quad (\text{equation S7})$$

$$\log (q_e - q_t) = \log q_e - \frac{k}{2.303} t \quad (\text{equation S8})$$

$$\frac{t}{q_t} = \frac{1}{h} + \frac{t}{q_e} \quad (\text{equation S9})$$

$$q_t = k_3 \cdot t^{0.5} \quad (\text{equation S10})$$

$$q_t = \frac{\ln a_e b_e}{b_e} + \frac{1}{b_e} \ln t \quad (\text{equation S11})$$

q_e = The amount of BPA adsorbed per unit mass of adsorbent (mg/g).

C_e = The equilibrium concentration of the solute in the bulk solution (mg/L).

q_{\max} = The maximum adsorption capacity.

K_L = Langmuir constant (b).

C_i = The initial concentration of the solution (mg/L)

B = The Temkin constant related to heat of sorption (J mol^{-1})

A_0 = The Temkin equilibrium binding constant (L/g)

β = The constant of the adsorption energy ($\text{mol}^2 \text{J}^{-2}$)

ε = Polanyi potential

R = The gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$)

T = The absolute temperature (K)

E = The value of mean energy of adsorption (kJ mol^{-1})

q_t = BPA adsorbed at time t (mg/g)

h = Initial sorption rate

k = The pseudo-second-order rate constant (g/mg.min)

k_3 = The intraparticle diffusion rate constant ($\text{mg.g}^{-1}.\text{min}^{-0.5}$)

a_e = The initial adsorption rate, $\text{mg (g}^{-1}.\text{min}^{-1})$

b_e = The extent of surface coverage

- 1 J. Ma, S. Li, G. Wu, M. Arabi, F. Tan, Y. Guan, J. Li and L. Chen, *J. Ind. Eng. Chem.*, 2020, **90**, 178-189.
- 2 M. Pan, X. Lin, J. Xie and X. Huang, *RSC advances*, 2017, **7**, 4492-4500.