

Absorption isotherm models

According to the linear and nonlinear Langmuir model, it was assumed that the adsorption energy is uniform and there is no adsorbate migration in the surface plane [1,2], and is expressed as in Eq (1) and (2):

$$C_e/q_e = 1/q_m K_L + C_e/q_m \quad (1)$$

$$q_e = q_m K_L C_e / (1 + K_L C_e) \quad (2)$$

where, “ q_e ” is the amount of solute adsorbed per unit weight of adsorbent at equilibrium (mg/g), “ C_e ” is the equilibrium concentration of the solute in bulk solution (mg/L), “ q_m ” is the maximum adsorption capacity (mg/g), and K_L is the Langmuir constant(L/mg).

The linear and nonlinear Freundlich models assumes heterogeneous surface energies and it becomes more heterogeneous as the value of the slope approaches zero [2-4]. Freundlich equation can be also written as Eq (3) and (4):

$$\ln q_e = \ln K_F + 1/n \ln C_e \quad (3)$$

$$q_e = K_F C_e^{1/n} \quad (4)$$

where, “ K_F ” is a constant indicative of the relative adsorption capacity of the adsorbent ($\text{mg}^{1-(1/n)}\text{L}^{1/n}/\text{g}$) and “ n ” is a constant indicative of the intensity of the adsorption, and “ C_e ” is the equilibrium concentration of the solute in bulk solution (mg/L).

According to the Temkin model, it was assumed that the adsorption heat of all molecules in the layer decreases linearly with the coverage area due to the adsorbent-adsorbate interactions and the adsorption is characterized by a homogeneous distribution of binding energies up to a maximum binding energy [5]. Equation can be written as follows Eq. (5):

$$q_e = RT/b \ln K_T + RT/b \ln C_e \quad (5)$$

where “ q_e ” is the amount of solute adsorbed per unit weight of adsorbent at equilibrium (mg/g), “ $RT/b = B$ ”, “ R ” is the gas constant (8.314 J/mol K), “ T ” is the absolute temperature in Kelvin unit, “ b ” is related to the heat of adsorption (J/mol), “ K_T ” is the Temkin constant (L/mg), and “ C_e ” the equilibrium concentration of the solute in bulk solution (mg/L).

The Elovich model is based on a kinetic principle, which is assumed to increase exponentially by adsorption regions, which indicates a multi-layer adsorption [4]. The equation of Elovich isotherm is as follows Eq. (6):

$$\ln(q_e/C_e) = \ln(K_E q_m) - 1/q_m q_e \quad (6)$$

where, “ q_e ” is the amount of solute adsorbed per unit weight of adsorbent at equilibrium (mg/g), “ C_e ” is the equilibrium concentration of the solute in bulk solution (mg/L), “ q_m ” is the maximum adsorption capacity (mg/g), and K_E is the Elovich constant (L/mg).

Dubinin-Radushkevich isotherm model is generally applied to express the adsorption mechanism on heterogeneous surfaces [6]. It is expressed by Eq. (7):

$$\ln q_e = \ln q_m - B \varepsilon^2 \quad (7)$$

where “ q_m ” represents the adsorption capacity (mg/g), “ R ” is the gas constant (8.314 J/molK), and “ T ” refers to the temperature as Kelvin. In addition, ε^2 value is given by $\varepsilon^2 = (RT \ln(1 + 1/C_e))^2$ equation.

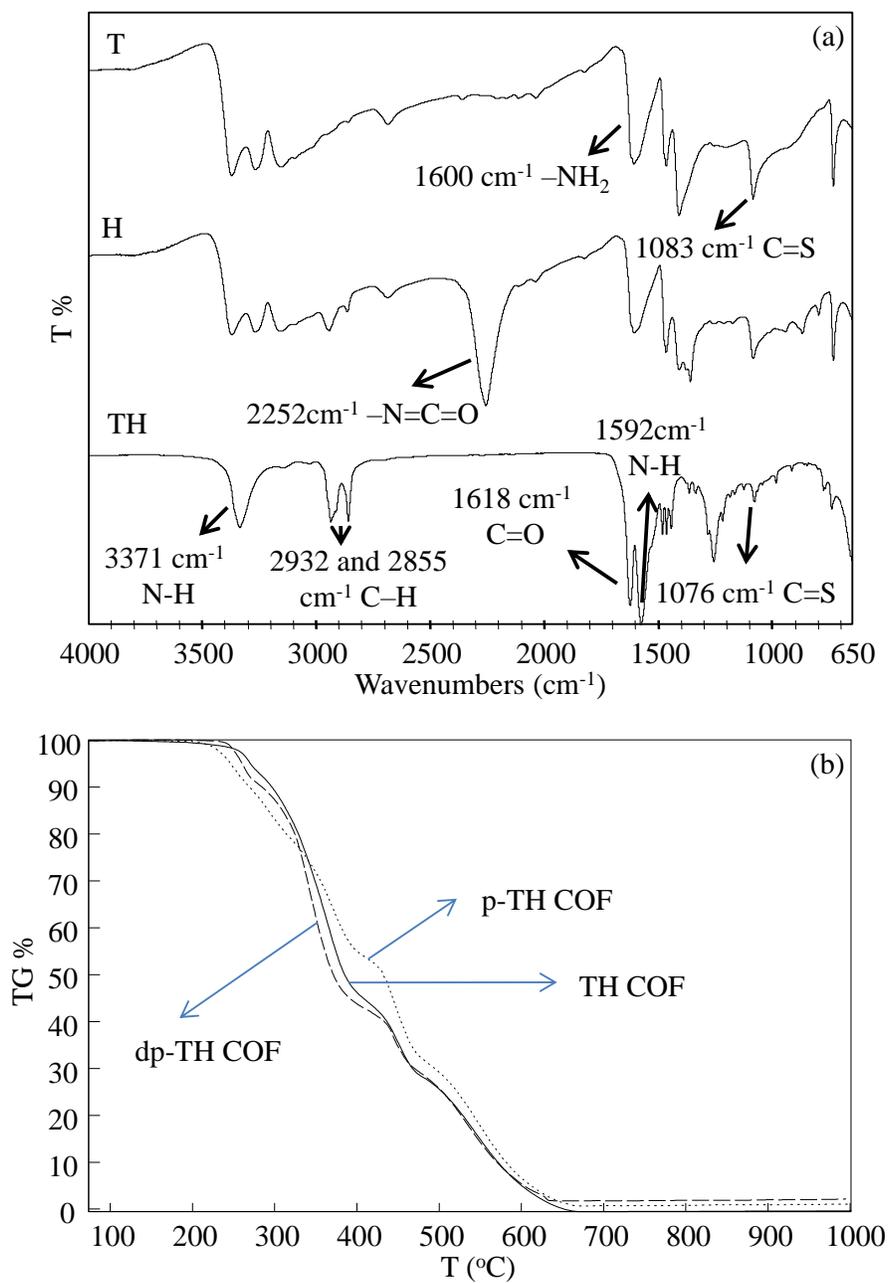


Figure S1. (a) FT-IR spectra and (b) TGA thermograms of TH based COFs.

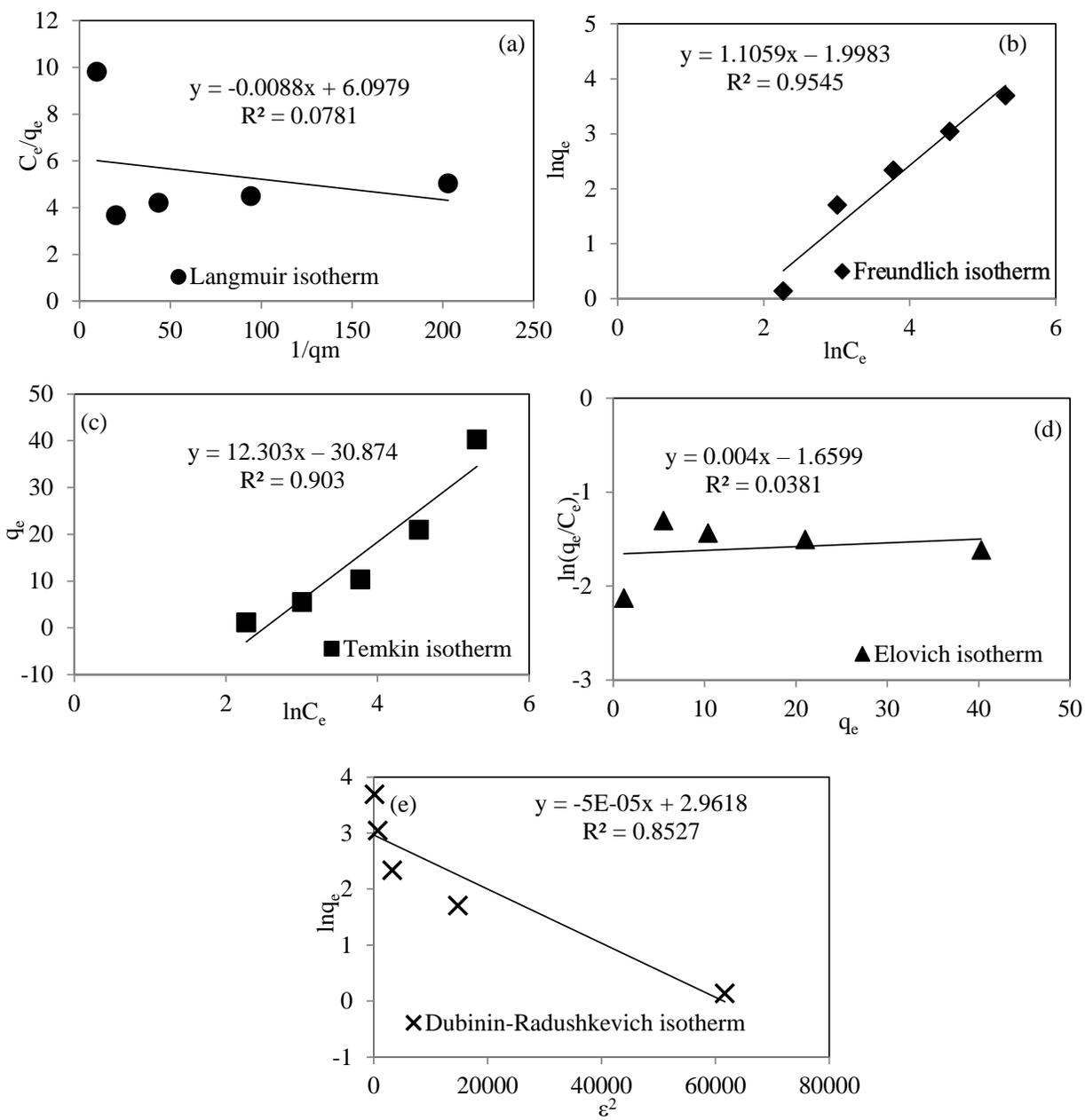


Figure S2. The (a) Langmuir, (b) Freundlich, (c) Temkin, (d) Elovich, and (e) Dubinin-Radushkevich isotherms for MB absorption by dp-TH COFs.

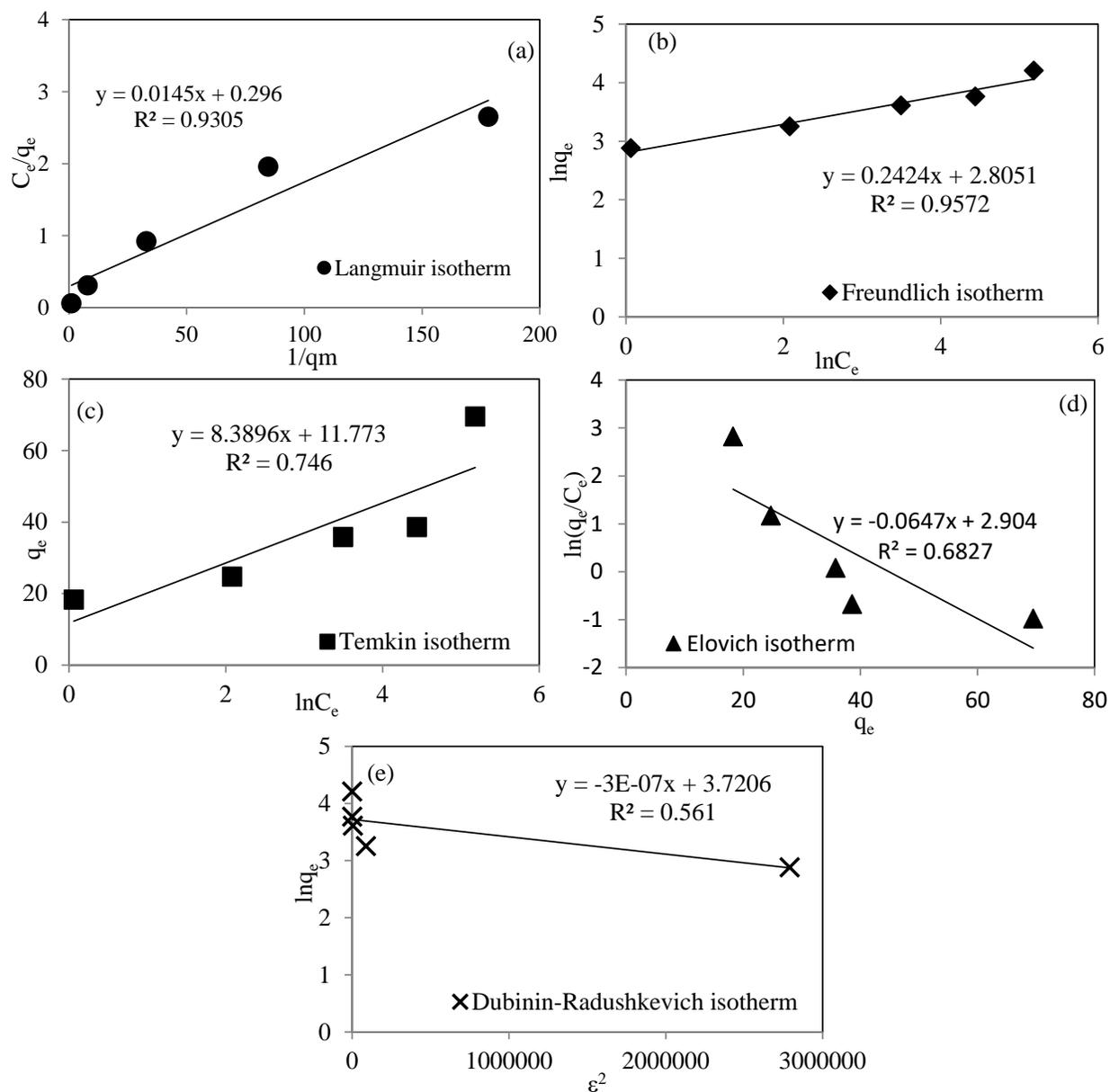


Figure S3. The (a) Langmuir, (b) Freundlich, (c) Temkin, (d) Elovich, and (e) Dubinin-Radushkevich for MO adsorption by p-TH COFs.

Table S1. Equilibrium pH values of 25 ppm 100 mL of MB and MO solutions at the end of absorption process by using TH, dp-TH, and p-TH COFs as absorbents and without absorbent.

Dye	pH values			
	Without absorbent	TH COF	dp-TH COF	p-TH COF
MB	6.2±0.3	6.6±0.1	8.7±0.3	-
MO	6.7±0.1	7.5±0.2	-	3.8±0.2

Table S2. Various isotherm constants for absorption of MB and MO dyes by dp-TH, and p-TH COFs, respectively.

Isotherm model	Isotherm constants				Situation
Langmuir (Linear)	Dye	K_L (L/mg)	q_m (mg/g)	R^2	
	MB	1×10^{-3}	113.6	0.078	Not fit
	MO	2×10^{-3}	68.9	0.930	Not fit
Langmuir (Nonlinear)	MB	9×10^{-4}	98.6	0.098	Not fit
	MO	2×10^{-1}	72.2	0.942	Not fit
Freundlich (Linear)	Dye	K_F ($\text{mg}^{1-(1/n)} \text{L}^{1/n} \text{g}^{-1}$)	n	R^2	
	MB	1×10^{-1}	0.91	0.954	Not fit
	MO	16.5	4.12	0.957	Not fit
Freundlich (Nonlinear)	MB	3×10^{-1}	1.01	0.998	Fit
	MO	17.5	3.83	0.998	Fit
Temkin	Dye	K_T (L/mg)	B (kJ mol ⁻¹)	R^2	
	MB	8×10^{-2}	204.8	0.903	Not fit
	MO	4.06	300.3	0.746	Not fit
Elovich	Dye	K_E (L/mg)	Q_m (mg/g)	R^2	
	MB	8×10^{-4}	250	0.038	Not fit
	MO	1.18	15.4	0.683	Not fit
Dubinin-Radushkevich	Dye	B (mol ² /kJ ²)	Q_m (mg/g)	R^2	
	MB	5×10^{-5}	19.3	0.853	Not fit
	MO	3×10^{-7}	41.3	0.561	Not fit

References

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