Supplementary Data

Optimizing methylene blue adsorption conditions on hydrothermally synthesized NaX zeolite through a full two-level factorial design

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Table S1. Experimental ranges of factors levels.

Factor	Coded factor	-1	1
pH	x_1	2	12
Solid/liquid ratio (S/L)	x_2	0.5	3.5
Initial concentration (C_0, mg/L)	x_3	5	120
Temperature (T, K)	x_4	298	333

Table S2. Elemental composition of NaX zeolite.

Element	(%) mass	(%) atomic
O	44.95	57.14
Na	15.27	13.51
Al	18.10	13.64
Si	21.69	15.71
Si/Al	1.198	1.152

Table S3. Non-linear and linear isotherm models used.

	Nonlinear form	Linear form	Plot
Models with two-parameters			
Langmuir-1	$q_e = \frac{q_{m\ L} K_L . C_e}{1 + K_L . C_e}$	$\frac{C_e}{q_e} = \frac{1}{q_m} C_e + \frac{1}{q_m b}$	C_e/q_e vs C_e
Freundlich	$q_e = K_F . C_e^{1/n}$	$\ln q_e = \ln K_F + \frac{1}{n} \ln C_e$	$\ln q_e$ vs $\ln C_e$
Temkin	$q_e = \frac{RT}{B_T} \ln K_T C_e$	$q_e = \frac{RT}{B_T} \ln K_T + \frac{RT}{B_T} \ln C_e$	q_e vs $\ln C_e$
Elovich	$\frac{q_e}{q_{mE}} = K_E C_e \exp\left(\frac{q_e}{q_{mE}}\right)$	$\ln \frac{q_e}{C_e} = \ln K_E q_{mE} - \frac{q_e}{q_{mE}}$	$\ln \frac{q_e}{C_e}$ vs q_e

Table S4. Mathematical expression of error functions used

Error function	Expression
Coefficient of determination, R^2	$R^2 = \frac{\sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})_i^2}{\sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})^2 + (q_{e.exp} - q_{e.cal})^2}$
Adjusted R-Squared	$R_{adj}^2 = 1 - \frac{(1 - R^2) * (n - 1)}{n - k - 1}$
Sum of squares errors, SSE:	$SSE = \sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})_i^2$
Reduced chi-square, χ^2	$\chi^2 = \frac{\sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})_i^2}{n - p}$
Mean Square Error, MSE	$MSE = \frac{100}{n-2}\sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})_i^2$
Root Mean Square Error, RMSE	$RMSE = \sqrt{\frac{100}{n-2}\sum_{i=1}^{n}(q_{e.exp} - q_{e.cal})_i^2}$
Akaike information criterion, AIC	$AIC = 2p + n * \ln(\frac{SSE}{n})$
Corrected evaluation of AIC, AICc	$AIC = 2p + n * \ln(\frac{SSE}{n}) + 2p * \frac{(p + 1)}{(n - p - 1)}$

Table S5. Separation factor (R_L) for MB adsorption onto NaX zeolite.

Concentration C (mg/L)	5	8	10	20	30	80	100	110	120
R_L=(1/(1+b*C))	0.62	0.51	0.45	0.29	0.22	0.14	0.09	0.07	0.06

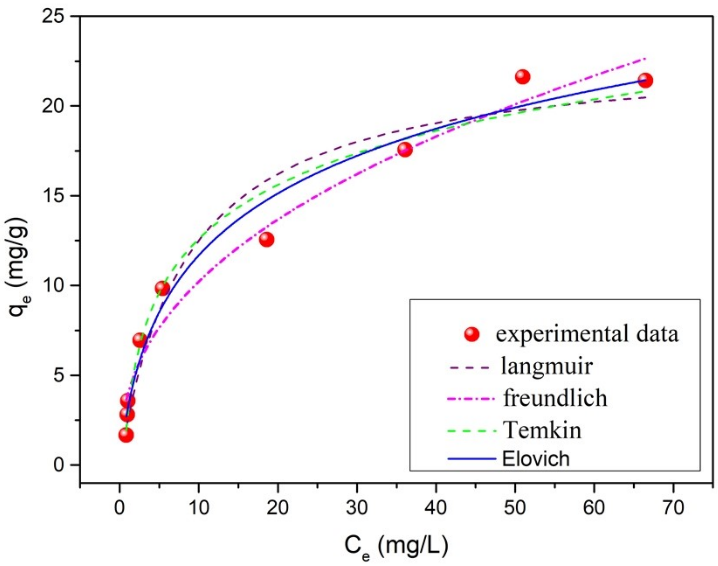

Figure S1. MB adsorption isotherms onto NaX using non-linear regression

(pH = 2, S/L = 2.5 g/L, and T = 298 K)

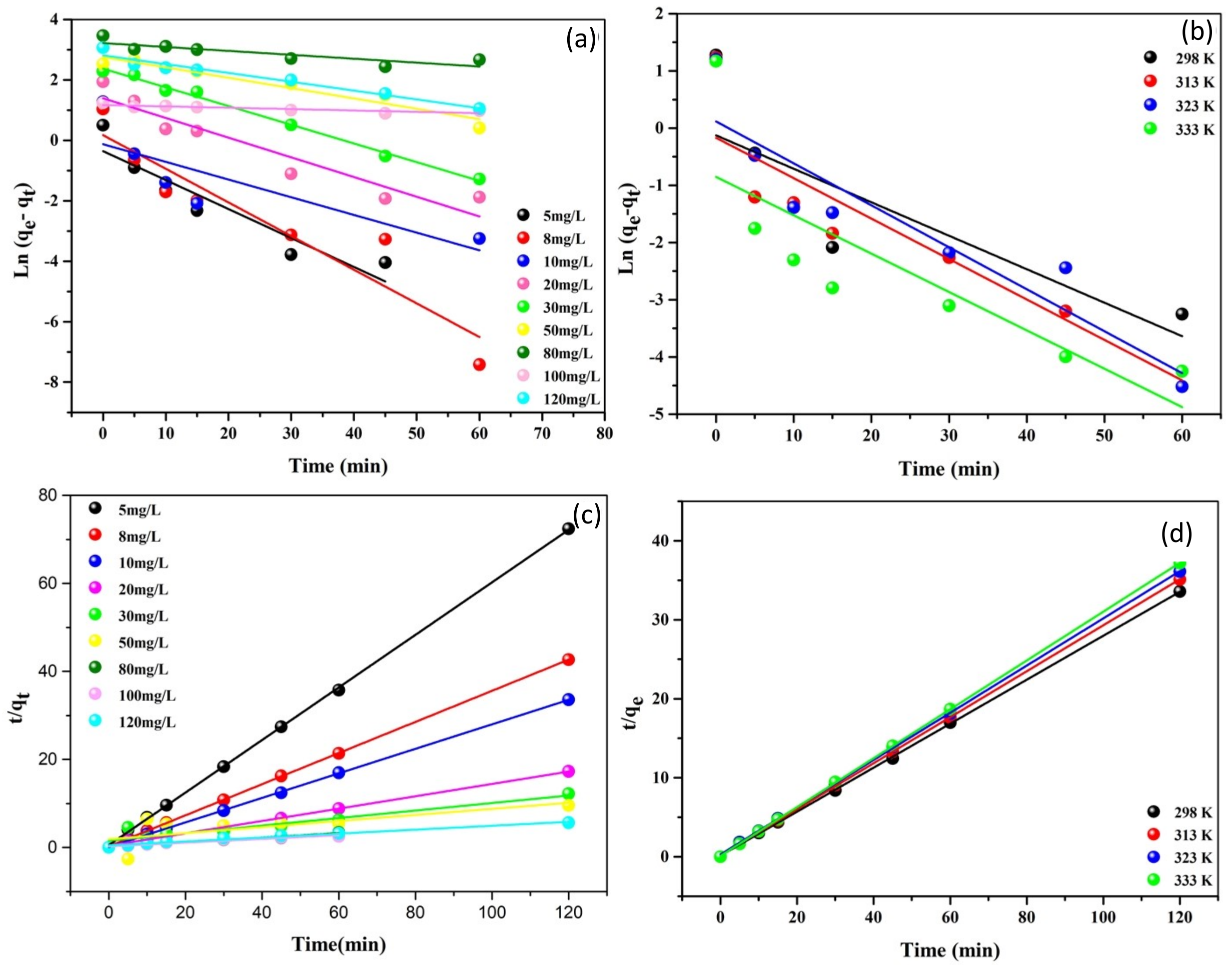

Figure S2. Pseudo-first-order kinetic models (a) at different concentrations, (b) at different temperatures, and pseudo-second-order kinetic models (c) at different concentrations, (d) at different temperatures for the MB adsorption onto the NaX zeolite.

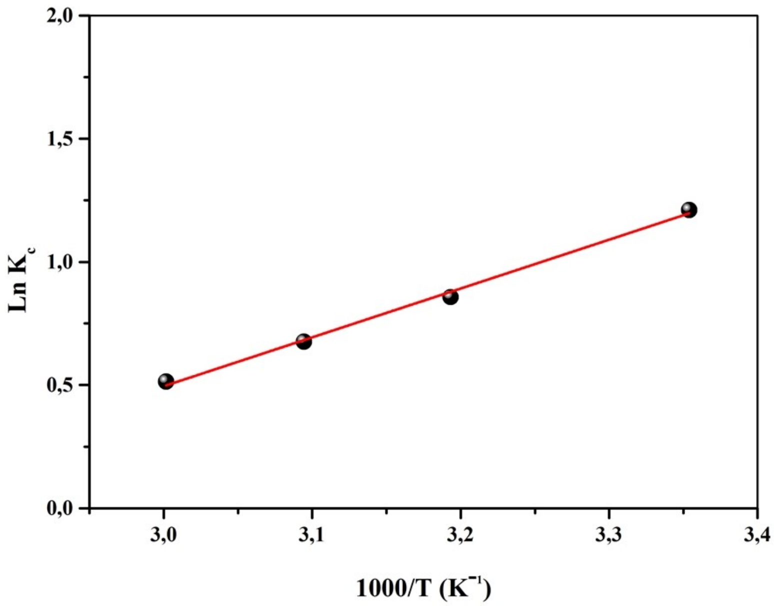

Figure S3. Plot of LnK_c as a function of (1000/T)

(C_0 = 10 mg/L, S/L = 2.5 g/L and pH = 2)