

Kinetics, Equilibrium, Statistical Surface Modeling and Cost Analysis of Paraquat Removal from Aqueous Solution using Carbonated Jujube Seed

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Supporting Information

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A) RSM Modeling procedure

In this part of work, Central Composite Design (CCD) coupled with Response Surface Methodology (RSM) ¹. were applied for seeking the optimum conditions for the adsorption of Paraquat onto JS/HSO-700 adsorbent. The complete design consisted of five-level (-2(- α), -1, 0, +1, +2(+ α)) and four-variable (Contact Time— X_1 , Temperature— X_2 , Initial Concentration— X_3 , pH— X_4). The ranges and levels of four variables namely Contact Time (CT), Temperature (T), Initial Concentration (IC), pH and the experiments matrix are given in **Table S2**. NEMRODW 2007 software ², was used for regression and graphical analysis of the data obtained.

To evaluate the effect of each independent variable on the paraquat removal (%), a second-order polynomial equation was used ³, which is expressed by the following **Equation 10**.

$$Y = a_0 + \sum_{i=1}^k a_i X_i + \sum_{i=1}^k a_{ii} X_i^2 + \sum_{i=1}^{k-1} \sum_{j=1}^k a_{ij} X_i X_j \quad (10)$$

Where y is the predicted response variable; a_0 is the constant coefficient; a_i is the linear coefficients; a_{ii} is the quadratic coefficients; a_{ij} is the linear coefficients for the interaction between independent variables i and j ; x_i and x_j are the coded independent parameters.

B) Figures

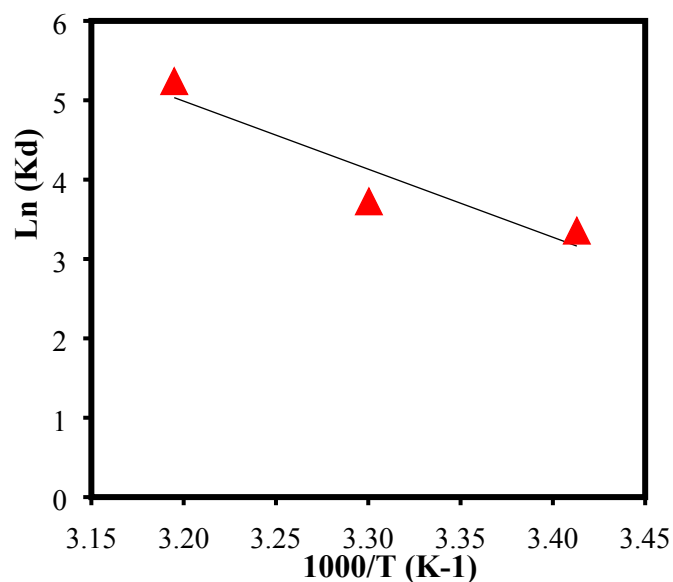


Figure S1: Van't Hoff plot for the adsorption of paraquat onto JS/HSO-700.

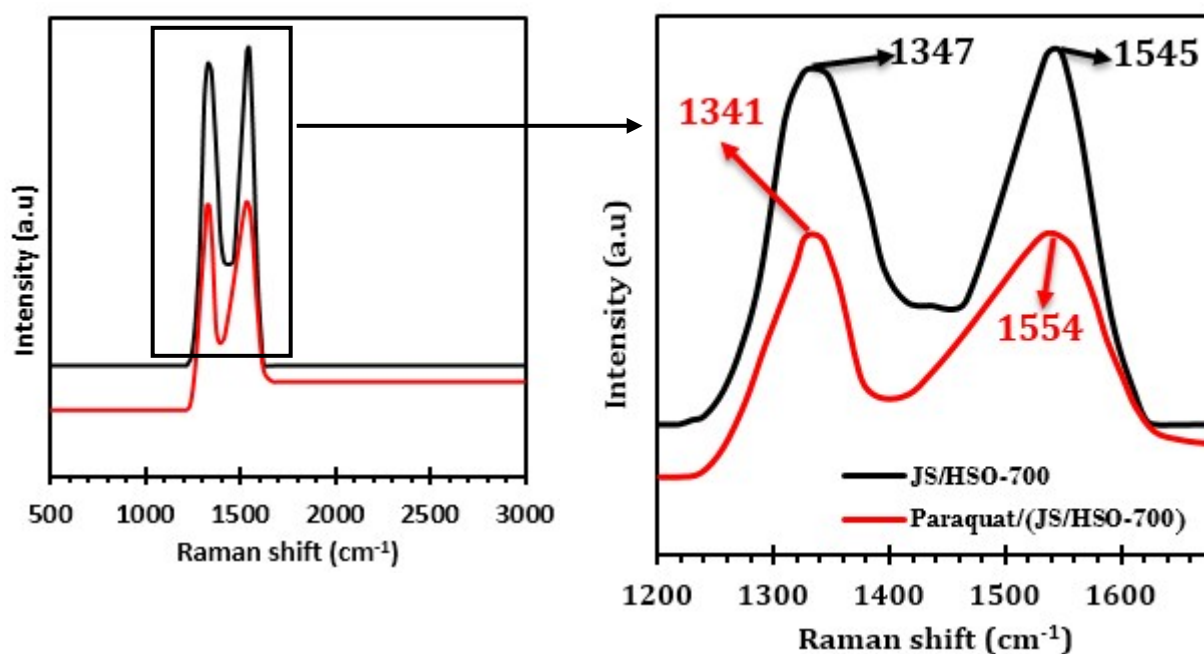


Figure S2 : Raman spectra of JS/HSO-700 after paraquat adsorption

C) Tables

Table S1: Textural properties of JS/HSO-700, without Paraquat-5th and with Paraquat-1st

Samples	S _{BET} (m ² /g)	VT (cm ³ /g)	Pores size (Å)
JS/HSO-700	973	0.75	39.3
Without Paraquat-5 th	706	0.53	39.4
With Paraquat-1 st	580	0.40	37.9

Table S2: Experimental domains of factors and CCD matrix

Variable	Name	Unit	-2 (α)	-1	0	+1	+2 (α)
X ₁	Contact time	min	10	17.5	25.00	32.5	40
X ₂	Temperature	K	293	298	303	308	313
X ₃	Initial concentration	mg/L	50	62.5	75	87.5	100
X ₄	pH	-	4	4.63	5.25	5.88	6.5
Run no.	Operating parameters				Response –R%–		
	Contact time (min)	Temperature (K)	Initial concentration (mg/L)	pH	Predicted		
1	-1.00000	-1.00000	-1.00000	-1.00000	60.17		
2	1.00000	-1.00000	-1.00000	-1.00000	75.24		
3	-1.00000	1.00000	-1.00000	-1.00000	68.59		
4	1.00000	1.00000	-1.00000	-1.00000	75.22		
5	-1.00000	-1.00000	1.00000	-1.00000	62.56		
6	1.00000	-1.00000	1.00000	-1.00000	75.82		
7	-1.00000	1.00000	1.00000	-1.00000	78.63		
8	1.00000	1.00000	1.00000	-1.00000	82.21		
9	-1.00000	-1.00000	-1.00000	1.00000	70.22		
10	1.00000	-1.00000	-1.00000	1.00000	85.25		
11	-1.00000	1.00000	-1.00000	1.00000	80.14		
12	1.00000	1.00000	-1.00000	1.00000	84.23		
13	-1.00000	-1.00000	1.00000	1.00000	74.66		
14	1.00000	-1.00000	1.00000	1.00000	91.23		
15	-1.00000	1.00000	1.00000	1.00000	86.55		
16	1.00000	1.00000	1.00000	1.00000	94.64		
17	- α	0.00000	0.00000	0.00000	66.19		
18	+ α	0.00000	0.00000	0.00000	82.63		
19	0.00000	- α	0.00000	0.00000	73.05		
20	0.00000	+ α	0.00000	0.00000	86.14		
21	0.00000	0.00000	- α	0.00000	84.16		
22	0.00000	0.00000	+ α	0.00000	85.82		
23	0.00000	0.00000	0.00000	- α	64.63		
24	0.00000	0.00000	0.00000	+ α	91.12		
25	0.00000	0.00000	0.00000	0.00000	83.43		
26	0.00000	0.00000	0.00000	0.00000	84.52		
27	0.00000	0.00000	0.00000	0.00000	78.08		
28	0.00000	0.00000	0.00000	0.00000	83.12		
29	0.00000	0.00000	0.00000	0.00000	80.43		
30	0.00000	0.00000	0.00000	0.00000	82.55		

Table S3. Significance of regression coefficients for Paraquat removal onto JS/HSO-700.

Sum of squares	Degrees of	Mean square	F-value	P-value
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freedom					
Regression	2.07333E+0003	14	1.48095E+0002	23.0493	< 0.0001
Residue	9.63774E+0001	15	6.42516E+0000		
Lack-of-fit	6.85967E+0001	10	6.85967E+0000	1.2346	0.432>0.05
Error	2.77807E+0001	5	5.55614E+0000		
Total	2.16971E+0003	29			
R ²	0.956				
R ² _{Adj}	0.914				
Coefficient		t.exp		P-value	
a_0	82.025	79.27		< 0.0001	
a_{CT}	4.798	9.27		< 0.0001	
a_T	3.387	6.55		< 0.0001	
a_{IC}	2.104	4.07		0.00101	
a_{pH}	5.905	11.41		< 0.0001	
a_{CT}^2	-2.142	-4.42		0.000492	
a_T^2	-0.845	-1.75		0.101	
a_{IC}^2	0.503	1.04		0.315	
a_{pH}^2	-1.278	-2.64		0.0185	
a_{CT-T}	-2.346	-3.70		0.00213	
a_{CT-IC}	0.043	0.07		0.947	
a_{T-IC}	1.279	2.02		0.062	
a_{CT-pH}	0.330	0.52		0.610	
a_{T-pH}	-0.416	-0.66		0.522	
a_{IC-pH}	0.459	0.72		0.480	

References

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