Supplementary Materials

Solvent-Free Mechanochemical Preparation of Metal-Organic Framework ZIF-67 Impregnated by Pt Nanoparticles for Water Purification

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The final regression model of 1 and 2, based on the encrypted values for the 4-NP reduction.

1. Y (Final Equation in Terms of Coded Factors) = 86.44 + 9.79A + 21.31B - 3.56C - 5.17AB - 7.15AC + 1.33BC - 5.22A^2 - 12.23B^2 - 3.98C^2

2. Y (Final Equation in Terms of Actual Factors) = - 541.35721 + (3.75091E+005) A + (43040.89444) B + (2.33010E+005) C – (7.31001E+006) AB – (8.08560E+007) AC + (1.88031E+006) BC – (5.90030E+007) A^2 – (2.16121E+006) B^2 – (4.49968E+007) C^2

The experimental layout was determined as a function of the most essential factors, including reducing agent concentration (A), catalyst value (B) and 4-NP concentration, for reaching the optimal conditions of eliminating 4-NP (Table S1).

Table S1. Experiments designed 20 performances with 3 variables.

		Facture	Facture	Facture
Std.	Run	A: $NaBH_4$ (M)	B: Catalyst (g)	C: 4-NP (M)
1	9	0.0012	0.003	0.0012
2	11	0.0017	0.003	0.0012
3	13	0.0012	0.008	0.0012
4	2	0.0017	0.008	0.0012
5	17	0.0012	0.003	0.0017
6	20	0.0017	0.003	0.0017
7	10	0.0012	0.008	0.0017
8	15	0.0017	0.008	0.0017
9	4	0.001	0.006	0.0015
10	18	0.002	0.006	0.0015
11	1	0.0015	0.002	0.0015
12	12	0.0015	0.01	0.0015
13	6	0.0015	0.006	0.001
14	8	0.0015	0.006	0.002
15	14	0.0015	0.006	0.0015
16	16	0.0015	0.006	0.0015
17	19	0.0015	0.006	0.0015
18	5	0.0015	0.006	0.0015
19	7	0.0015	0.006	0.0015
20	3	0.0015	0.006	0.0015

The p-value of this model is 0.0001, and the high F-value equals 14.70, indicating the importance of the selected model and the effect of changing the selected variable on the nitro reduction rate response. As a result, our model is statistically significant and acceptable. In most statistical software, the "probability value" (p-value) is applied to facilitate the decision about the result of the statistical hypothesis test. This value helps you decide whether to reject the null hypothesis without looking at the statistical distribution tables. F-value can also be used to determine whether the test is statistically significant. The F-value is used in the analysis of variance (ANOVA) for the probability of a significant value for the test. Factors A, B, AC, and B^2 have p-values less than 0.05; therefore, they are critical to purity (Table S2). Also, according to Table S1, it is important to check another parameter, i.e. Lack of Fit, for the model. This parameter includes zero and alternative statistical hypotheses. Therefore, according to the table below, this parameter is statistically unacceptable and shows Lack of Fit. In general, if the value for a defined model is P-value > Lack of Fit, then a fit model would be available. These factors are critical to express the percentage of purity.

Table S2. Standard Deviation Analysis (ANOVA) of data obtained for nitro reduction rate.

Analysis of variance table [Partial sum of squares - Type III]						
Source	**Sum of Squares**	**df**	**Mean Square**	**F-Value**	p-value Prob> F	
Model	10795.76	9	1199.53	14.70	0.0001	significant
A-$NaBH_4$	1309.62	1	1309.62	16.05	0.0025	
B-cat.	6204.65	1	6204.65	76.05	< 0.0001	
C-p-nitro	173.31	1	173.31	2.12	0.1756	
AB	213.75	1	213.75	2.62	0.1366	
AC	408.61	1	408.61	5.01	0.0492	
BC	14.14	1	14.14	0.17	0.6860	
A^2	391.96	1	391.96	4.80	0.0532	
B^2	2154.01	1	2154.01	26.40	0.0004	
C^2	227.96	1	227.96	2.79	0.1256	
Residual	815.84	10	81.58			
Lack of Fit	579.15	5	115.83	2.45	0.1742	not significant
Pure Error	236.70	5	47.34	Pure Error		
Cor Total	11611.60	19				

In addition, based on the value of R-square (R^2) = 0.92 (detection coefficient) and R^2-adjusted = 0.86, the adjusted detection coefficient shows the appropriate overlap of the obtained data and the values predicted by the model (Table S3). The closer the R^2 is to one, the more statistically valid the model is.

Table S3. Data and the values predicted by the model.

R-squared correlation (R^2)	**0.92**
R^2-adjusted correlation	0.86
R^2-predicted correlation	0.59

Usually, for reaching to the normal distribution, the obtained data is normalized to look like a direct line. However, the correlation factor is normally used to define the degree of correlation between the model and the experimental data. In other view, the suggested model shows a considerable correlation, including parameters valuable in reducing and deleting 4-NP. In Figure S1, a series of 3-D response surfaces for checking the parameters A-B, A-C and B-C, demonstrate the simultaneous consequences of binary parameters at the reaction variables (Figure 7).

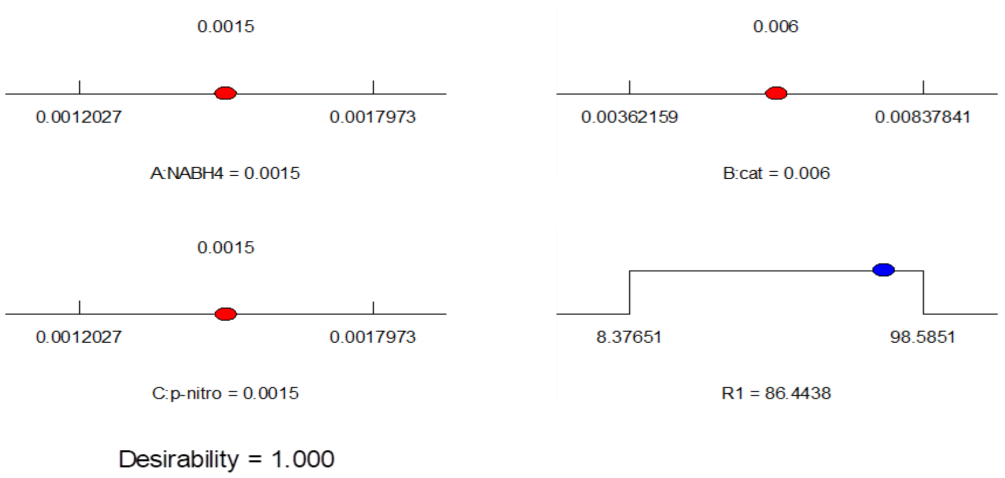

Figure S1. The results obtained and conformity the expected values of the model.