

Bimetallic Cu-Fe₃O₄ nanocomposite-loaded nanocellulose: a magnetic catalyst for reductive elimination of toxic nitroarenes from water; Optimization using response surface methodology

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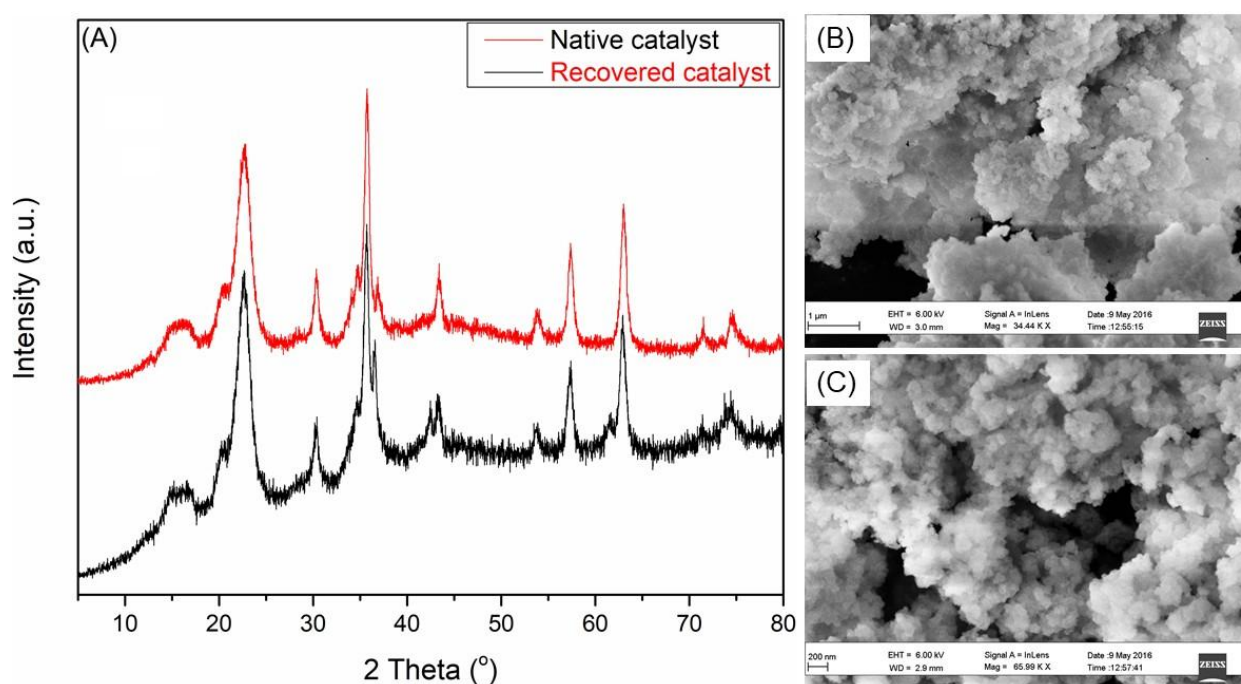


Figure S1

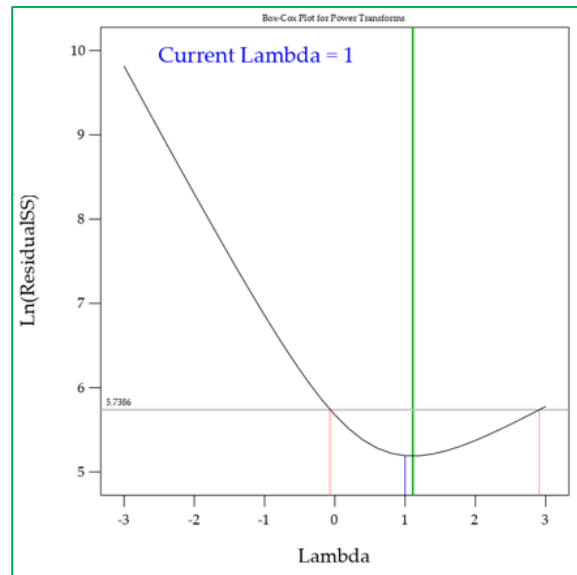


Figure S1. Power transformation using box-cox plot.

Table S1: Experimental factors and their coded and actual levels used in the response surface methodology optimization.

No.	Factors			Levels and Codes			Dependent variables		
	Factor	Symbol	Unit	−1	0	+1	Parameter (Unit)	Symbol	Objective
1	Catalyst dose	A	mg	5	10	15	Conversion of NB to AB (%)	Y	Maximize
2	NaBH ₄	B	Equivalent	1	2	3			
3	Temperature	C	°C	25	75	100			

Table S2: Experimental design matrix and observed response values for the catalytic reduction of nitrobenzene.

Run	Catalyst (mg)	NaBH ₄ (equiv)	Temp (°C)	Conversion (%)
1	5	1	75	82.0
2	5	3	75	93.0
3	15	1	75	88.0
4	15	3	75	96.0
5	5	2	25	30.0
6	5	2	100	80.0
7	15	2	25	45.0
8	15	2	100	93.0
9	10	1	25	28.0
10	10	1	100	86.0
11	10	3	25	40.0
12	10	3	100	95.0
13	10	2	75	98.5
14	10	2	75	94.5
15	10	2	75	85.0
16	10	2	75	96.0
17	10	2	75	92.0

Table S3: Analysis of variance (ANOVA) for the quadratic response surface methodology model.**Response 1: Conversion of NB to AB**

Source	Sum of Squares	df	Mean Squares	F- value	P-value	
Model	9664.51	9	1073.83	41.75	< 0.0001	Significant
A-Catalyst dose	171.13	1	171.13	6.65	0.0365	
B-NaBH ₄	200.00	1	200.00	7.78	0.0270	
C-Temperature	5565.13	1	5565.13	216.36	< 0.0001	
AB	2.25	1	2.25	0.0875	0.7760	
AC	1.0000	1	1.0000	0.0389	0.8493	
BC	2.25	1	2.25	0.0875	0.7760	
A ²	14.41	1	14.41	0.5603	0.4785	
B ²	10.78	1	10.78	0.4191	0.5380	
C ²	3627.04	1	3627.04	141.01	< 0.0001	
Residual	180.05	7	25.72			Not significant
Lack of Fit	73.75	3	24.58	0.9251	0.5057	
Pure Error	106.30	4	26.57			
Cor Total	9844.56	16				
Std. Dev.	5.07		R ²		0.9817	
Mean	77.76		Adjusted R ²		0.9582	
CV %	6.52		Predicted R ²		0.8633	
			Adeq precision		17.6103	

Table S3: continue

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Mean vs Total	1.028E+05	1	1.028E+05			
Linear vs Mean	5936.25	3	1978.75	6.58	0.0061	
2FI vs Linear	5.50	3	1.83	0.0047	0.9995	
Quadratic vs 2FI	3722.76	3	1240.92	48.24	< 0.0001	Suggested
Cubic vs Quadratic	73.75	3	24.58	0.9251	0.5057	Aliased
Residual	106.30	4	26.57			
Total	1.126E+05	17	6626.44			

Table S3: continue**Coefficients in Terms of Coded Factors**

Factor	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
Intercept	93.20	1	2.27	87.84	98.56	
A-Catalyst dose	4.63	1	1.79	0.3850	8.86	1.0000
B-NaBH ₄	5.00	1	1.79	0.7600	9.24	1.0000
C-Temperature	26.38	1	1.79	22.14	30.61	1.0000
AB	-0.7500	1	2.54	-6.75	5.25	1.0000
AC	-0.5000	1	2.54	-6.50	5.50	1.0000
BC	-0.7500	1	2.54	-6.75	5.25	1.0000
A ²	-1.85	1	2.47	-7.69	3.99	1.01
B ²	-1.60	1	2.47	-7.44	4.24	1.01
C ²	-29.35	1	2.47	-35.19	-23.51	1.01

Table S4. Process optimization criteria.

Constraint name	Units	Goal	Limits		Weights		Importance
			lower	upper	lower	upper	
A: Catalyst dose	mg	is in range	-1	1	1	1	3
B: NaBH ₄	Equivalent	is in range	-1	1	1	1	3
C: Temperature	°C	is in range	-1	1	1	1	3
Conversion of NB to AB	%	maximize	28	98.5	1	1	3