

**Optimization of the process parameters for the adsorption of ternary dyes by Ni doped
FeO(OH)-NWs-AC using response surface methodology and artificial neural network**

Farshid Nasiri Azad ^a, Mehrorang Ghaedi ^{*a}, Arash Asfaram ^a, Arsalan Jamshidi ^{b, c}, Ghasem Hassani ^{b, c},
Alireza Goudarzi ^d, Mohammad Hossein Ahmadi Azqhandi ^e, Abdolmohammad Ghaedi ^f

^a Chemistry Department, Yasouj University, Yasouj 75918-74831, Iran

^b Department of Environmental health engineering, Faculty of public health, Yasouj University of medical
sciences, Yasouj, Iran

^c Social determinates of health research center Yasouj University of medical sciences, Yasouj, Iran

^d Department of Polymer Engineering, Golestan University, Gorgan, 49188-88369, Iran

^e Applied Chemistry Department, Faculty of Gas and Petroleum (Gachsaran), Yasouj University,
Gachsaran, 75918-74831, Iran

^f Chemistry Department, Gachsaran Branch, Islamic Azad University, Gachsaran 75818-63876, Iran

* Corresponding authors: Mehrorang Ghaedi

Tel/fax: Fax: +98-741-2223048

E-mail: m_ghaedi@mail.yu.ac.ir; m_ghaedi@yahoo.com

32 **Table S1.** Analysis of variance (ANOVA) for the dyes adsorption.

Source of variation	Df ^a	% R CG				% R RB				% R DB			
		SS ^b	MS ^c	F-value	P-value	SS	MS	F-value	P-value	SS	MS	F-value	P-value
Model	27	9309.5	344.77	81.987	< 0.0001	10630	393.69	1050.31	<0.0001	5144.4	190.54	113.747	< 0.0001
A	1	856.98	856.98	203.76	< 0.0001	459.65	459.65	1226.28	<0.0001	429.25	429.25	256.254	< 0.0001
B	1	798.80	798.80	189.94	< 0.0001	978.59	978.59	2610.72	<0.0001	363.42	363.42	216.957	< 0.0001
C	1	146.89	146.89	34.928	0.001975	241.78	241.78	645.032	<0.0001	13.834	13.834	8.25859	0.03484
D	1	161.28	161.28	38.350	0.001602	153.30	153.30	408.981	<0.0001	22.646	22.646	13.5196	0.01434
E	1	717.83	717.83	170.69	< 0.0001	759.33	759.33	2025.78	<0.0001	431.59	431.59	257.655	< 0.0001
F	1	32.000	32.000	7.6091	0.03991	50.000	50.000	133.392	<0.0001	93.571	93.571	55.8608	0.000677
AB	1	124.71	124.71	29.655	0.002836	334.71	334.71	892.947	<0.0001	97.318	97.318	58.0977	0.000618
AC	1	334.43	334.43	79.522	0.000295	161.93	161.93	431.991	<0.0001	132.37	132.37	79.0202	0.000299
AD	1	288.86	288.86	68.685	0.000418	1679.6	1679.6	4480.98	<0.0001	210.51	210.51	125.669	< 0.0001
AE	1	8.1758	8.1756	1.9441	0.2220	250.71	250.71	668.856	<0.0001	29.547	29.547	17.6394	0.008490
AF	1	20.318	20.316	4.8312	0.07929	144.72	144.72	386.093	<0.0001	19.936	19.936	11.9017	0.01824
BC	1	480.00	480.00	114.14	0.000124	849.06	849.07	2265.20	<0.0001	529.08	529.08	315.851	< 0.0001
BD	1	40.673	40.673	9.6712	0.02655	6.4516	6.4516	17.2119	0.00892	37.149	37.149	22.1775	0.005293
BE	1	590.37	590.37	140.38	< 0.0001	79.924	79.924	213.224	<0.0001	332.70	332.70	198.616	< 0.0001
BF	1	302.66	302.66	71.966	0.000374	161.85	161.85	431.783	<0.0001	195.37	195.37	116.636	0.000118
CD	1	4.2539	4.2539	1.0115	0.3607	7.8961	7.8961	21.0656	0.0059	7.4256	7.4256	4.4330	0.08913
CE	1	33.034	33.034	7.8549	0.03787	160.02	160.02	426.915	<0.0001	14.063	14.063	8.39513	0.03389
CF	1	529.41	529.41	125.88	< 0.0001	859.37	859.37	2292.66	<0.0001	255.95	255.95	152.798	< 0.0001
DE	1	787.24	787.24	187.19	< 0.0001	1063.0	10630	2835.8	<0.0001	465.13	465.13	277.678	< 0.0001
DF	1	247.67	247.67	58.891	0.000599	86.583	86.583	230.99	<0.0001	384.36	384.36	229.455	< 0.0001
EF	1	80.147	80.147	19.058	0.007253	742.29	742.29	1980.32	<0.0001	23.814	23.814	14.2169	0.01302
A ²	1	367.99	367.99	87.503	0.000235	7.7260	7.7260	20.6117	0.00617	282.25	282.25	168.502	< 0.0001
B ²	1	233.30	233.30	55.476	0.000688	806.11	806.11	2150.57	<0.0001	214.89	214.89	128.289	< 0.0001
C ²	1	139.15	139.15	33.088	0.002228	3.2845	3.2845	8.76246	0.03151	78.182	78.182	46.6734	0.001025
D ²	1	1071.8	1071.8	254.86	< 0.0001	135.65	135.65	361.894	<0.0001	19.521	19.521	11.6536	0.01897
E ²	1	40.229	40.229	9.5659	0.02707	0.0903	0.0903	0.24099	0.6443	13.872	13.872	8.28143	0.03468
F ²	1	1502.5	1502.5	357.26	< 0.0001	1659.9	1659.9	4428.49	<0.0001	683.49	683.49	408.035	< 0.0001
Residual	5	21.028	4.2055			1.8742	0.3748			8.3754	1.6751		
Lack of Fit	1	12.424	12.424	5.7766	0.07408	1.0351	1.0351	4.93441	0.09048	0.2498	0.2498	0.12297	0.7435
Pure Error	4	8.6032	2.1508			0.8391	0.2098			8.1256	2.0314		
Cor Total	32	9330.5				10631				5152.8			

33 ^a Degree of freedom, ^b Sum of Square, ^c Mean of Square.

34 **Table. S2.** Quality of quadratic model based on R², CV% and SD.

Response	R% CG	R% RB	R% DB
Coefficient of variation (CV %)	3.960	1.181	3.281
Standard deviation (SD)	2.051	0.6122	1.294
Adequate precision (AP)	34.83	137.4	44.22
Mean	51.78	51.83	39.45
R-Squared (R ²)	0.9977	0.9998	0.9984
Adj R-Squared (Adj-R ²)	0.9856	0.9989	0.9896

35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59

60 **Table S3.** Dependence among neuron number at hidden layer, MSE and R²

NO. neurons	CG				RB				DB			
	Train		Test		Train		Test		Train		Test	
	MSE	R ²	MSE	R ²	MSE	R ²	MSE	R ²	MSE	R ²	MSE	R ²
1	0.000104	0.997869	0.005041	0.831757	0.000565	0.988798	0.009590	0.576922	0.000188	0.008668	0.996276	0.654262
2	0.000094	0.998072	0.077629	0.987409	0.000076	0.998491	0.002895	0.872278	0.000076	0.099568	0.998491	0.879928
3	0.000094	0.998072	0.007763	0.994091	0.000074	0.998541	0.009307	0.958941	0.000076	0.006290	0.998491	0.872278
4	0.000097	0.998020	0.005525	0.999724	0.000073	0.998552	0.008674	0.961734	0.000076	0.008531	0.998487	0.838476
5	0.000095	0.998054	0.001945	0.965082	0.000041	0.999987	0.003325	0.999906	0.000076	0.007843	0.998487	0.891176
6	0.000093	0.998109	0.002068	0.930988	0.000074	0.998539	0.008304	0.942457	0.000093	0.004699	0.999981	0.999602
7	0.000093	0.998104	0.002116	0.929373	0.000073	0.998555	0.007407	0.937915	0.000113	0.007261	0.997472	0.998040
8	0.000093	0.998104	0.002135	0.928754	0.000076	0.998500	0.004477	0.934861	0.000076	0.007252	0.997926	0.950111
9	0.000092	0.998111	0.002433	0.918782	0.000076	0.998500	0.006330	0.897222	0.000093	0.007246	0.997927	0.939381
10	0.000093	0.998107	0.002553	0.914797	0.000080	0.998411	0.005358	0.895996	0.000093	0.072435	0.997928	0.938865
11	0.000104	0.997869	0.005041	0.831757	0.000188	0.996276	0.007830	0.654555	0.000093	0.005243	0.997927	0.938860
12	0.008640	0.823445	0.007481	0.750322	0.000077	0.998465	0.009506	0.889437	0.008783	0.002142	0.803596	0.801206
13	0.004545	0.907130	0.008972	0.700550	0.000079	0.998429	0.004910	0.871603	0.000188	0.004252	0.996276	0.654016
14	0.000099	0.997980	0.009234	0.691804	0.000176	0.996514	0.008531	0.623665	0.000093	0.004261	0.997929	0.938610
15	0.005172	0.894311	0.011471	0.617142	0.000078	0.998449	0.005722	0.747567	0.000093	0.004270	0.996167	0.937923
16	0.005173	0.894302	0.011480	0.616860	0.000079	0.998428	0.004934	0.870556	0.000565	0.004272	0.998449	0.796293
17	0.005177	0.894223	0.011489	0.616537	0.000079	0.998427	0.004949	0.869894	0.000093	0.004364	0.996276	0.783982
18	0.005180	0.894163	0.011514	0.615709	0.000077	0.998463	0.004897	0.783982	0.000093	0.004399	0.996274	0.751878
19	0.005182	0.894112	0.011517	0.615631	0.000193	0.996167	0.005624	0.751878	0.000092	0.004403	0.996276	0.747567
20	0.005181	0.894144	0.011518	0.615594	0.000081	0.998389	0.003123	0.862235	0.000188	0.004618	0.996276	0.653818
21	0.005184	0.894075	0.011518	0.615585	0.000076	0.998497	0.003168	0.860248	0.000239	0.004897	0.996276	0.807836
22	0.005187	0.894010	0.011558	0.614242	0.000188	0.996274	0.007824	0.654840	0.000092	0.005624	0.996276	0.654555
23	0.005205	0.893636	0.011575	0.613696	0.000082	0.998382	0.004185	0.815374	0.000093	0.005722	0.996514	0.654262
24	0.005192	0.893910	0.011577	0.613615	0.000078	0.998449	0.004186	0.815319	0.000092	0.007820	0.996549	0.654016
25	0.005202	0.893695	0.011591	0.613157	0.000078	0.998449	0.004190	0.815173	0.000093	0.007824	0.988798	0.653818

61

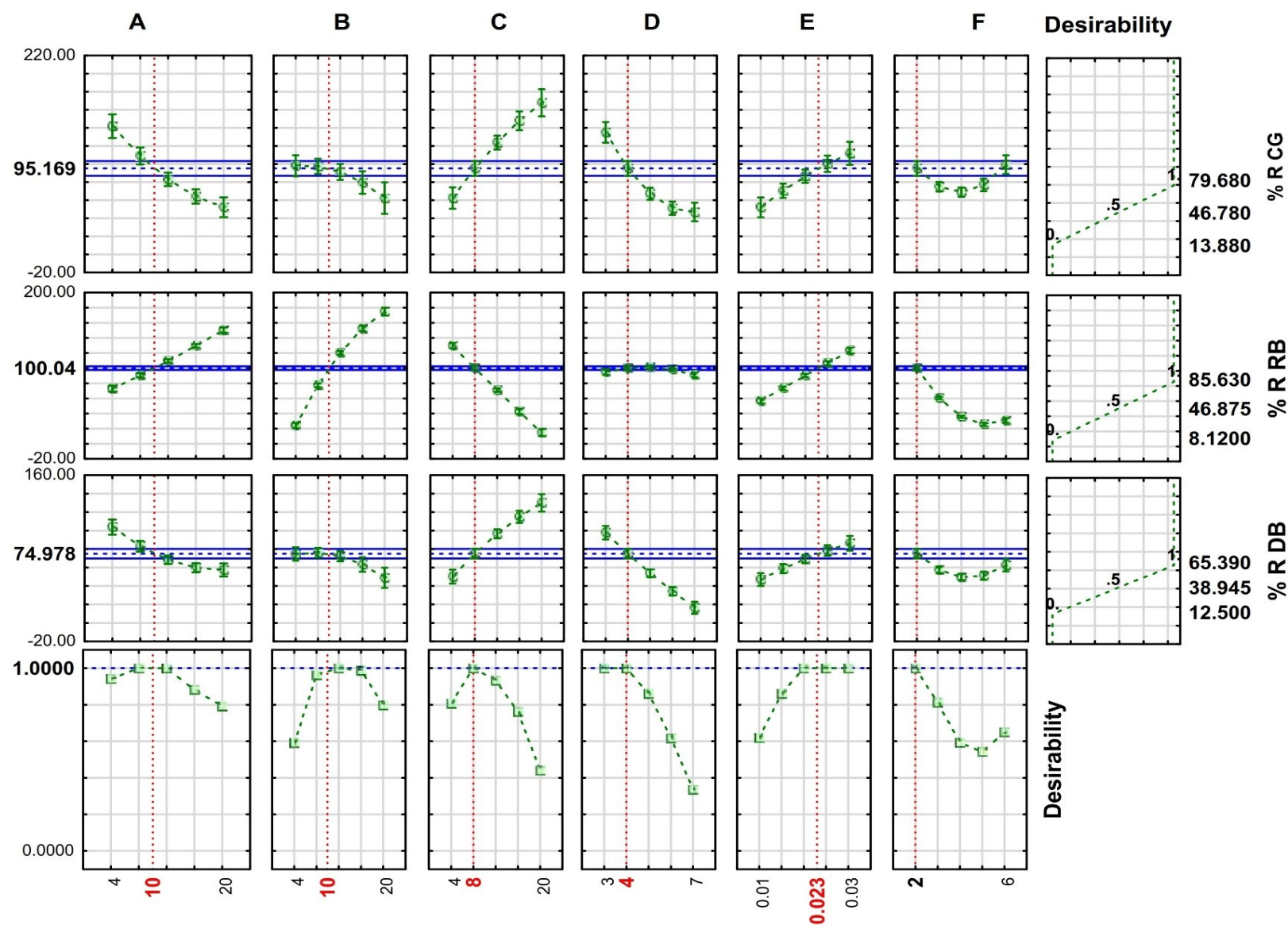
62

63

64

Table S4. Kinetic parameters for the adsorption of dyes using 0.010 g Ni doped FeO(OH)-NWs-AC as well as 15 mg L⁻¹ of each dye in single component.

Model	Parameters	CG	RB	DB
First-order- kinetic	k_1 (min ⁻¹)	0.216	0.111	0.125
	q_e (calc) (mg g ⁻¹)	13.690	12.30	7.890
	R^2	0.950	0.822	0.861
Pseudo-second-order-kinetic	k_2 (min ⁻¹)	0.009	0.0178	0.0145
	q_e (calc) (mg g ⁻¹)	86.350	112.630	115.350
	R^2	0.996	0.999	0.999
Intraparticle diffusion	K_{diff} (mg g ⁻¹ min ^{-1/2})	7.490	1.360	2.340
	C (mg g ⁻¹)	9.350	11.730	10.770
	R^2	0.986	0.963	0.973
Elovich	β (mg g ⁻¹ min ⁻¹)	0.363	1.530	2.607
	α (g mg ⁻¹)	239.630	325.101	210.20
	R^2	0.985	0.926	0.922
Experimental Data	q_e (exp) (mg g ⁻¹)	80.79	109.54	112.36



77
 78 **Fig. S1.** Profiles for predicated values and desirability function for removal percentage of CG, RB and DB. Dashed line indicates current values
 79 after the optimization.

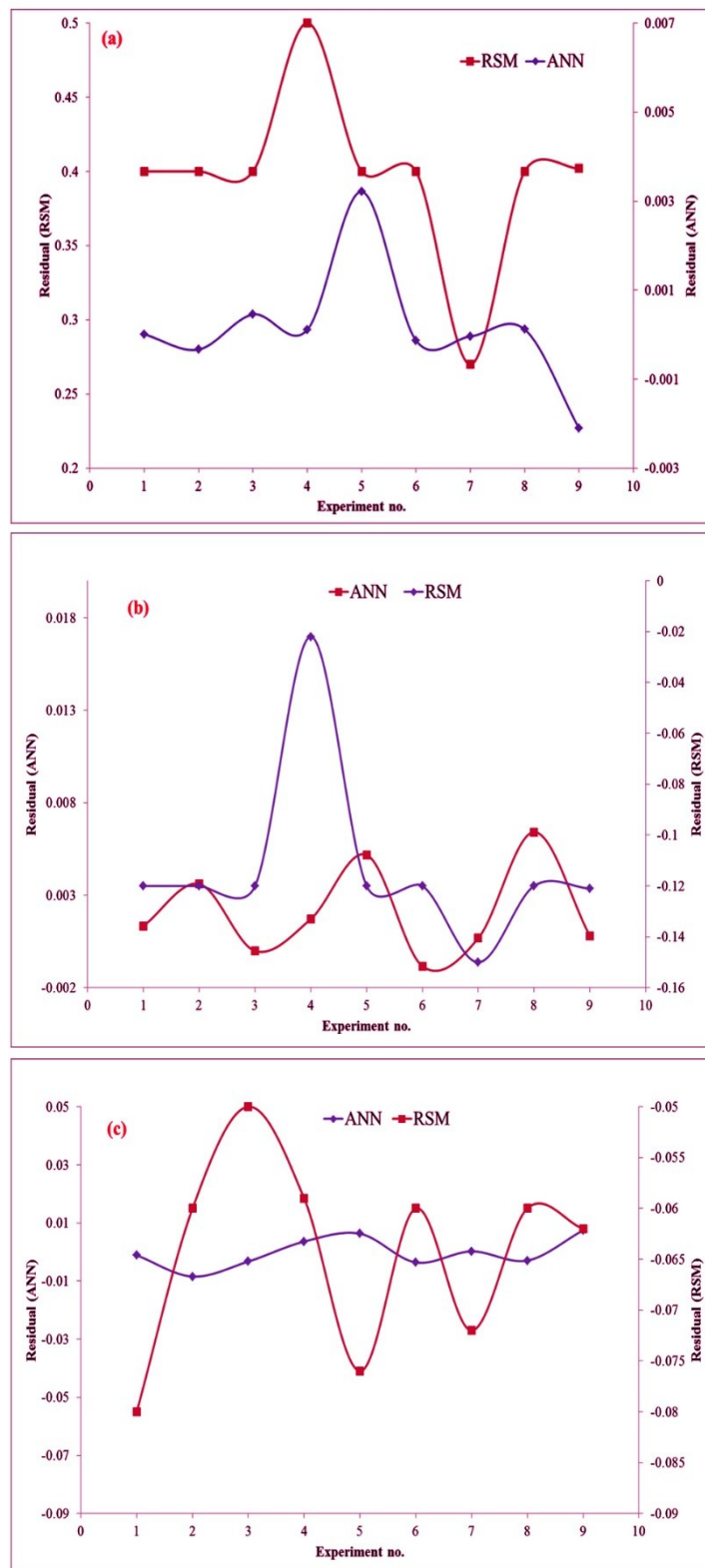


Fig. S2. Distribution of residuals, (a): CG; (b): RB; (c): BD