

Supplementary Information

Understanding and Predicting the Environmental Dispersion of Iron Oxide Nanoparticles: A Comprehensive Study on Synthesis, Characterisation, and Modelling.

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Table S1 – Coded values (x_1 : temperature, x_2 : time, x_3 : hardness, x_4 : pH) and Iron Content in Hematite Nanoparticles (HemNPs) Dispersion studied in experimental design.

Assays	x_1	x_2	x_3	x_4	Rep. 1	Rep. 2	Rep. 3	Mean
1	-1	-1	-1	-1	51.31	47.76	47.93	49 (± 2)
2	-1	+1	-1	-1	60.86	60.24	58.90	60 (± 1)
3	+1	-1	-1	-1	30.75	34.31	30.95	32 (± 2)
4	+1	+1	-1	-1	82.06	81.38	76.56	80 (± 3)
5	-1	-1	+1	-1	21.42	25.25	22.33	23 (± 2)
6	-1	+1	+1	-1	54.52	53.74	50.74	53 (± 2)
7	+1	-1	+1	-1	37.06	39.06	37.89	38 (± 1)
8	+1	+1	+1	-1	168.6	158.9	161.5	163 (± 5)
9	-1	-1	-1	+1	37.27	31.60	36.13	35 (± 3)
10	-1	+1	-1	+1	13.12	15.09	13.79	14 (± 1)
11	+1	-1	-1	+1	31.72	32.54	28.74	31 (± 2)
12	+1	+1	-1	+1	66.34	63.37	71.29	67 (± 4)
13	-1	-1	+1	+1	30.11	31.79	34.10	32 (± 2)
14	-1	+1	+1	+1	47.47	49.74	43.79	47 (± 3)
15	+1	-1	+1	+1	35.33	41.25	37.43	38 (± 3)
16	+1	+1	+1	+1	141.9	138.1	146.0	142 (± 4)
17	-2	0	0	0	6.36	5.31	6.33	6.0 (± 0.6)
18	+2	0	0	0	75.54	80.71	80.76	79 (± 3)
19	0	-2	0	0	3.66	4.23	4.11	4.0 (± 0.3)
20	0	+2	0	0	86.37	89.17	79.46	85 (± 5)
21	0	0	-2	0	162.6	156.4	155.1	158 (± 4)
22	0	0	+2	0	213.4	203.6	207.0	208 (± 5)
23	0	0	0	-2	50.45	47.81	51.74	50 (± 2)
24	0	0	0	+2	30.14	28.56	28.29	29 (± 1)
25	0	0	0	0	73.73	72.46	69.81	72 (± 2)
26	0	0	0	0	70.43	74.25	71.32	72 (± 2)
27	0	0	0	0	70.32	73.25	69.43	71 (± 2)
28	0	0	0	0	73.48	72.79	69.73	72 (± 2)
29	0	0	0	0	69.74	73.55	72.71	72 (± 1)
30	0	0	0	0	73.28	70.18	69.54	72 (± 2)
31	0	0	0	0	70.32	73.25	69.43	71 (± 2)

Table S2 – Regression equations in uncoded units for HemNPs dispersions: full model and reduced model with significant terms (x_1 : temperature, x_2 : time, x_3 : hardness, and x_4 : pH).

Full Quadratic CCRD	Regression Equations in Uncoded Units for HemNPs dispersion
All terms	$-508 + 16.05 x_1 - 3.29 x_2 - 1.821 x_3 + 168.5 x_4 - 0.414 x_1^2 - 0.0752 x_2^2 + 0.002405 x_3^2 - 11.70 x_4^2 + 0.2872 x_1 x_2 + 0.02504 x_1 x_3 - 1.019 x_1 x_4 + 0.00901 x_2 x_3 + 0.118 x_2 x_4 + 0.0361 x_3 x_4$
Significative terms	$-436 + 8.92 x_1 - 2.46 x_2 - 1.569 x_3 + 158.2 x_4 - 0.414 x_1^2 - 0.0752 x_2^2 + 0.002405 x_3^2 - 11.70 x_4^2 + 0.2872 x_1 x_2 + 0.02504 x_1 x_3 + 0.00901 x_2 x_3$

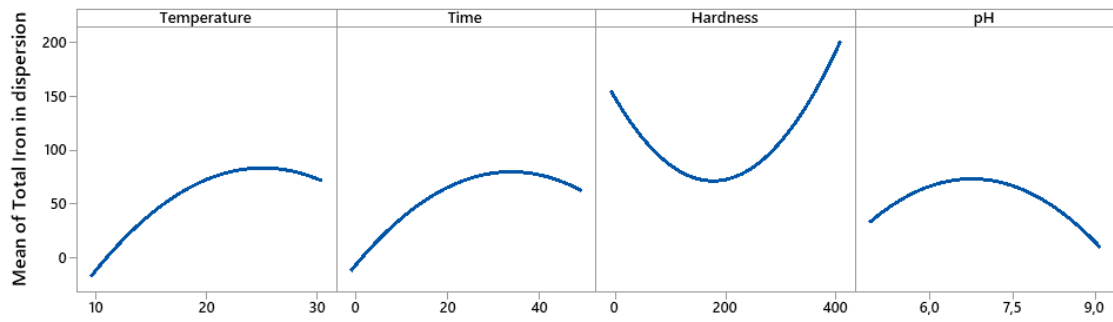


Figure S1 – Main effects plot for Total Iron in Hematite nanoparticles dispersions with all model terms included.

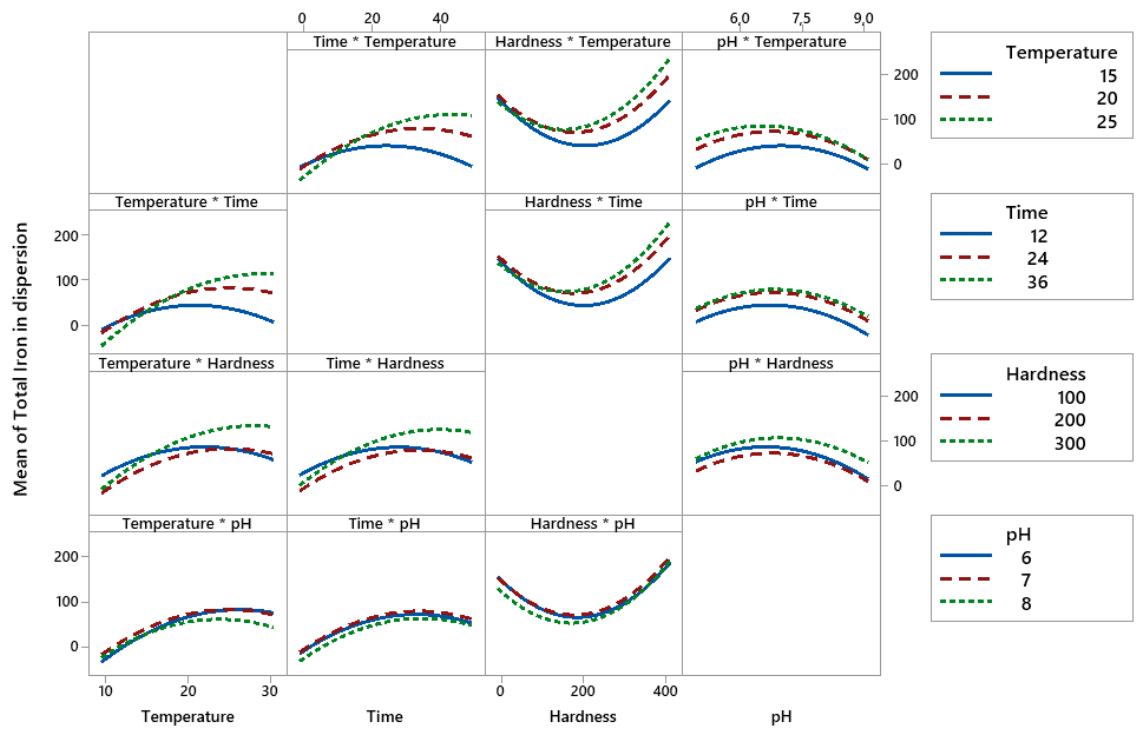


Figure S2 – Interaction plot for Total Iron in Hematite nanoparticle dispersions with all model terms included.

Table S3 – Coded values (x_1 : temperature, x_2 : time, x_3 : hardness, x_4 : pH) and Iron Content in Goethite Nanoparticles (GoeNPs) Dispersion studied in experimental design.

Assays	x_1	x_2	x_3	x_4	Rep. 1	Rep. 2	Rep. 3	Mean
1	-1	-1	-1	-1	230.9	230.1	228.9	230 (\pm 1)
2	-1	+1	-1	-1	281.7	271.7	277.6	277 (\pm 5)
3	+1	-1	-1	-1	144.8	151.6	144.6	147 (\pm 4)
4	+1	+1	-1	-1	245.4	248.3	253.3	249 (\pm 4)
5	-1	-1	+1	-1	242.5	247.5	247.9	246 (\pm 3)
6	-1	+1	+1	-1	334.1	331.8	330.1	332 (\pm 2)
7	+1	-1	+1	-1	171.2	171.1	167.7	170 (\pm 2)
8	+1	+1	+1	-1	280.3	277.0	276.7	278 (\pm 2)
9	-1	-1	-1	+1	202.4	207.5	202.1	204 (\pm 3)
10	-1	+1	-1	+1	313.0	309.7	313.3	312 (\pm 2)
11	+1	-1	-1	+1	171.6	179.5	176.9	176 (\pm 4)
12	+1	+1	-1	+1	214.4	209.5	209.0	211 (\pm 3)
13	-1	-1	+1	+1	198.0	200.0	196.0	198 (\pm 2)
14	-1	+1	+1	+1	284.6	277.5	277.9	280 (\pm 4)
15	+1	-1	+1	+1	172.6	169.7	164.7	169 (\pm 4)
16	+1	+1	+1	+1	256.7	260.0	260.3	259 (\pm 2)
17	-2	0	0	0	415.5	421.5	423.0	420 (\pm 4)
18	+2	0	0	0	317.5	308.3	316.2	314 (\pm 5)
19	0	-2	0	0	26.97	25.05	22.97	25 (\pm 2)
20	0	+2	0	0	174.1	166.1	169.8	170 (\pm 4)
21	0	0	-2	0	489.7	495.5	493.8	493 (\pm 3)
22	0	0	+2	0	521.3	523.5	527.2	524 (\pm 3)
23	0	0	0	-2	132.0	133.0	131.0	132 (\pm 1)
24	0	0	0	+2	108.7	111.8	112.5	111 (\pm 2)
25	0	0	0	0	477.5	485.0	483.5	482 (\pm 4)
26	0	0	0	0	492.3	496.2	493.6	494 (\pm 2)
27	0	0	0	0	472.4	473.3	476.3	474 (\pm 2)
28	0	0	0	0	478.9	480.8	480.4	480 (\pm 1)
29	0	0	0	0	484.6	482.8	484.5	484 (\pm 1)
30	0	0	0	0	493.4	488.6	488.0	490 (\pm 3)
31	0	0	0	0	481.4	488.7	487.9	486 (\pm 4)

Table S4 – Regression equations in uncoded units for GoeNPs dispersions: full model and reduced model with significant terms (x_1 : temperature, x_2 : time, x_3 : hardness, and x_4 : pH).

Full Quadratic CCRD	Regression Equations in Uncoded Units for GoeNPs dispersion
All terms	$- 6205 + 173.5 x_1 + 6.65 x_2 + 0.376 x_3 + 1371.4 x_4 - 4.132 x_1^2 - 0.2501 x_2^2 - 0.000062 x_3^2 - 97.40 x_4^2 + 0.016 x_1 x_2 + 0.0091 x_1 x_3 - 0.36 x_1 x_4 + 0.00308 x_2 x_3 + 0.319 x_2 x_4 - 0.0755 x_3 x_4$
Significative terms	$- 6139 + 173.09 x_1 + 9.79 x_2 + 1355.9 x_4 - 4.130 x_1^2 - 0.2496 x_2^2 - 97.33 x_4^2$

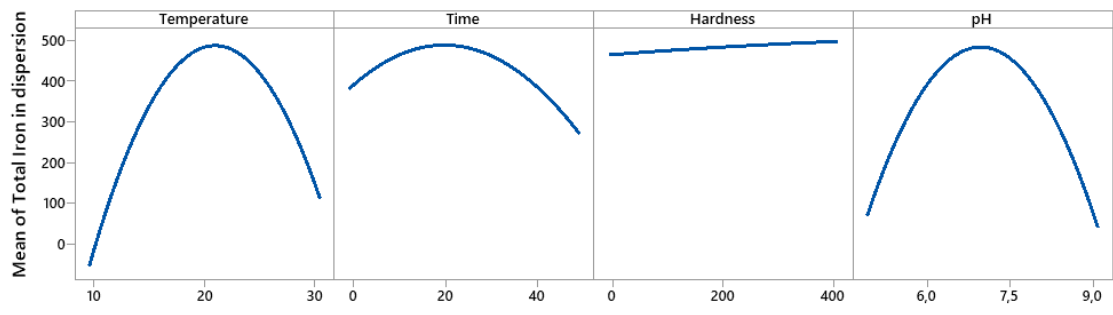


Figure S3 – Main effects plot for Total Iron in Goethite nanoparticles dispersions with all model terms included.

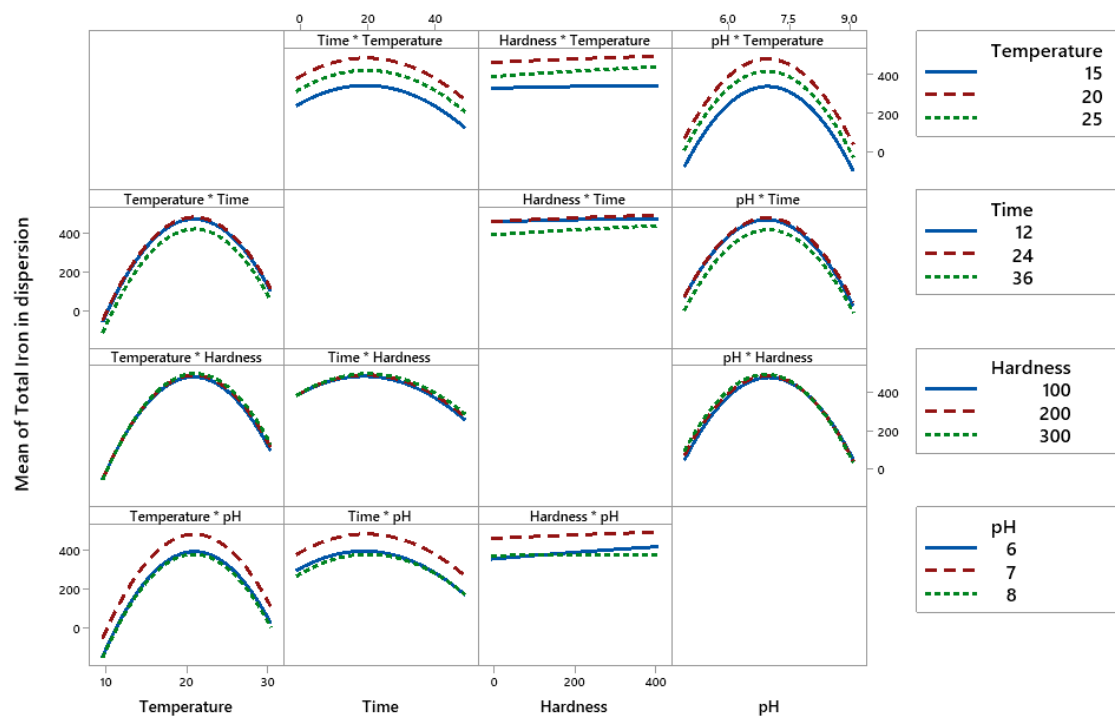


Figure S4 – Interaction plot for Total Iron in Goethite nanoparticle dispersions with all model terms included.

Table S5 – Coded values (x_1 : temperature, x_2 : time, x_3 : hardness, x_4 : pH) and Iron Content in Magnetite Nanoparticles (MagNPs) dispersion studied in experimental design.

Assays	x_1	x_2	x_3	x_4	Rep. 1	Rep. 2	Rep. 3	Mean
1	-1	-1	-1	-1	565.7	566.3	563.0	565 (± 3)
2	-1	+1	-1	-1	552.2	549.7	546.0	549 (± 4)
3	+1	-1	-1	-1	764.2	755.8	769.0	763 (± 9)
4	+1	+1	-1	-1	743.6	739.1	741.3	741 (± 8)
5	-1	-1	+1	-1	507.2	509.7	510.1	509 (± 5)
6	-1	+1	+1	-1	479.8	481.3	476.9	479 (± 3)
7	+1	-1	+1	-1	601	602.5	601.7	602 (± 2)
8	+1	+1	+1	-1	556.5	552	557.4	556 (± 4)
9	-1	-1	-1	+1	548.6	551	550.4	550 (± 5)
10	-1	+1	-1	+1	581.5	577.8	577.6	579 (± 6)
11	+1	-1	-1	+1	710.3	711.5	706.2	710 (± 7)
12	+1	+1	-1	+1	740.8	736.1	737.0	738 (± 9)
13	-1	-1	+1	+1	552.5	548.1	546.4	549 (± 6)
14	-1	+1	+1	+1	559	563.3	557.7	560 (± 5)
15	+1	-1	+1	+1	600.4	603.6	596.0	600 (± 4)
16	+1	+1	+1	+1	603.8	606.2	602.1	604 (± 2)
17	-2	0	0	0	101.4	103.7	101.0	102 (± 2)
18	+2	0	0	0	352.1	354.7	349.8	352 (± 3)
19	0	-2	0	0	10.73	8.91	10.4	10 (± 1)
20	0	+2	0	0	0	0	0.0	0 (± 1)
21	0	0	-2	0	1203.8	1211.7	1199.5	1205 (± 9)
22	0	0	+2	0	1027.2	1021.7	1024.4	1025 (± 8)
23	0	0	0	-2	1056.2	1064.4	1052.7	1058 (± 8)
24	0	0	0	+2	1092.4	1096.9	1090.1	1093 (± 6)
25	0	0	0	0	1103.5	1104.8	1097.7	1102 (± 7)
26	0	0	0	0	1100.1	1104.2	1095.8	1100 (± 6)
27	0	0	0	0	1098.4	1099.1	1099.6	1099 (± 8)
28	0	0	0	0	1102.7	1099.4	1100.2	1101 (± 6)
29	0	0	0	0	1100.8	1102.0	1097.2	1100 (± 7)
30	0	0	0	0	1103.2	1104.7	1099.1	1102 (± 9)
31	0	0	0	0	1100.8	1097.3	1105.2	1102 (± 6)

Table S6 – Regression equations in uncoded units for MagNPs dispersions: full model with all terms (x_1 : temperature, x_2 : time, x_3 : hardness, and x_4 : pH).

Full Quadratic CCRD	Regression Equations in Uncoded Units for MagNPs dispersion
All terms	$ \begin{aligned} & -4344.4 + 424.90 x_1 + 88.638 x_2 - 0.7380 x_3 + 47.76 x_4 - 10.9737 x_1^2 - 1.51973 x_2^2 + 0.000316 x_3^2 \\ & - 6.704 x_4^2 - 0.03125 x_1 x_2 - 0.01000 x_1 x_3 + 2.325 x_1 x_4 - 0.023125 x_2 x_3 - 0.7604 x_2 x_4 \\ & + 0.13000 x_3 x_4 \end{aligned} $

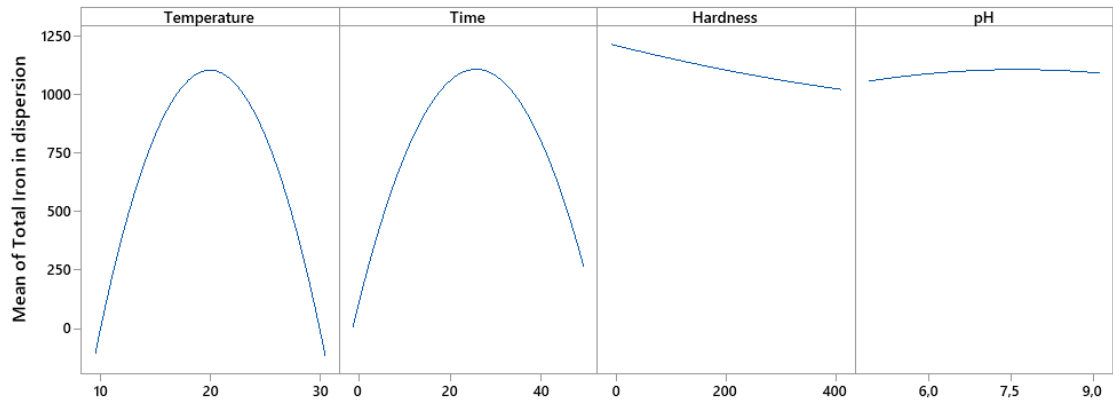


Figure S5 – Main effects plot for Total Iron in Magnetite nanoparticles dispersions with all model terms included.

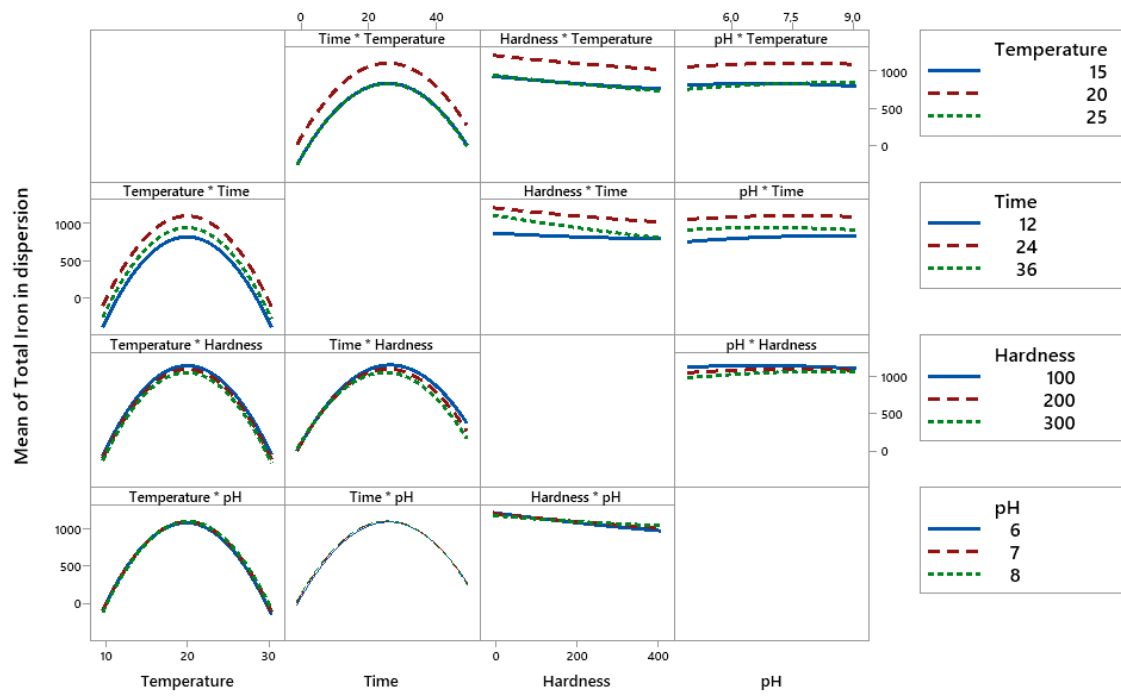


Figure S6 – Interaction plot for Total Iron in Magnetite nanoparticle dispersions with all model terms included.