

Supplementary data

Table 1.

Parameter	Sample		
	MNPs	PAC	MNPs@C
Average pore diameter (nm)	3.6	5.24	3.5
Pore volume (cm ³ /g)	0.006	0.753	0.487
Specific surface area (BET) (m ² /g)	63.26	936	671.2
Pore structure	Mesopore	Micropore	Mesopore
Color	Black	Black	Black

Table 2.

The values of kinetic constants of the COD removal from PCW by MNPs@C/H₂O₂ system
(conditions: pH 3.0, 1.0 g/L MNPs@C, 5.0 mM H₂O₂, and T=20±1°C)

Kinetic models	Parameter	Catalyst loading (g/L)					
		0.1	0.25	0.5	1	1.5	5
Zero-order	k	6.784	7.931	8.516	9.532	9.207	9.377
C = C ₀ - kt	SSE	1.117e+4	3.667e+4	5.21e+4	8.086e+4	8.731e+4	8.5e+4
	R ²	0.9099	0.8078	0.7733	0.7335	0.704	0.7171
	R ² adj	0.8874	0.7597	0.7166	0.6669	0.63	0.6463
	RMSE	52.84	95.75	114.1	142.2	147.7	145.8
First-order	k	0.01363	0.02411	0.03191	0.05138	0.0502	0.056
C = C ₀ exp(-kt)	SSE	5347	1.326e+4	1.478e+4	1.145e+4	1.855e+4	1.027e+4
	R ²	0.9569	0.9305	0.9357	0.9623	0.9371	0.9658
	R ² adj	0.9461	0.9131	0.9196	0.9528	0.9214	0.9573
	RMSE	36.56	57.58	60.79	53.5	68.09	50.66
Second-order	k	2.503e-5	5.538e-5	7.435e-5	0.000117	0.000113	0.000131
C = (C ₀)/1+ktC ₀	SSE	3147	2235	2026	6822	6602	1256
	R ²	0.9746	0.9883	2026	0.9775	0.9776	0.9958
	R ² adj	0.9683	0.9854	0.989	0.9719	0.972	0.9948
	RMSE	28.05	23.64	22.5	41.3	40.63	17.72
							32.66

Kinetic models	Parameters	H ₂ O ₂ dosage (mM)					
		5	25	50	100	200	500
Zero-order	k	6.293	7.927	9.524	9.146	7.576	6.373
C = C ₀ - kt	SSE	7.646e+4	7.474e+4	8.053e+4	7.917e+4	1.096e+5	9.799e+4
	R ²	0.5592	0.6732	0.734	0.7214	0.562	0.5039
	R ² adj	0.449	0.5915	0.6675	0.6517	0.4526	0.3799
	RMSE	138.3	136.7	141.9	140.7	165.5	156.5
First-order	k	0.02427	0.03557	0.0513	0.05281	0.05197	0.03166
C = C ₀ exp(-kt)	SSE	4.953e+4	3.158e+4	1.143e+4	1.374e+4	0.8218	6.132e+4
	R ²	0.7145	0.8619	0.9623	0.9516	4.458e+4	0.6895
	R ² adj	0.6431	0.8274	0.9528	0.9396	0.7773	0.6119
	RMSE	111.3	88.85	53.45	58.61	105.6	123.8
Second-order	k	7.244e-5	9.061e-5	0.000117	0.000128	0.00013	0.00013
C = (C ₀)/1+ktC ₀	SSE	2.25e+4	8500	6653	558.4	1.17e+4	2.363e+4
	R ²	0.8703	0.9628	0.978	0.998	0.9532	0.8804
	R ² adj	0.8379	0.9535	0.9725	0.9975	0.9416	0.8504
	RMSE	75	46.1	40.78	11.82	54.08	76.86

Table 3.

Lists of the coefficients of determination and error functions.

goodness of fit criteria	Abbreviation	Definition/expression
Determination coefficient	R ²	$R^2 = \frac{\sum_{i=1}^n (q_{i,\text{exp}} - \bar{q}_{i,\text{exp}})^2 - \sum_{i=1}^n (q_{i,\text{exp}} - q_{i,\text{calc}})^2}{\sum_{i=1}^n (q_{i,\text{exp}} - \bar{q}_{i,\text{exp}})^2}$
Adjusted determination coefficient	R ² adj	$R_{adj}^2 = 1 - (1 - R^2) \left(\frac{n-1}{n-p} \right)$
Sum squared error	SSE	$SSE = \sum_{i=1}^n (q_{i,\text{calc}} - q_{i,\text{exp}})^2$
Root mean square error	RMSE	$RMSE = \sqrt{\frac{\sum_{i=1}^n (q_{i,\text{exp}} - q_{i,\text{calc}})^2}{n}}$