

SUPPLEMENTARY MATERIAL TO

Comparison of the advanced oxidation processes in the degradation of pharmaceuticals and pesticides in simulated urban wastewater: Principal component analysis and energy requirements

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Text S1

All mobile phases were prepared volumetrically from individually measured aliquots and were degassed for 15 min in an ultrasonic bath before use. A mixture of phosphate buffer and acetonitrile (53:47, v/v) was used as a mobile phase for the determination of atenolol. Detection was carried out using a detector at 230 nm (Kumar et al., 2010). Atrazine was monitored at the wavelength of 220 nm and the isocratic mobile phase was pure acetonitrile and purified water (60:40, v/v) (Atarodia and Faghihiana, 2019). The chromatographic conditions used for cyprodinil were as follows: eluent A, water; eluent B, acetonitrile; gradient, 35–60% B over the first 3.5 min and then was stable for 20 min. The chromatograms were performed at 280nm (Vaquero-Fernandez et al., 2008). The mobile phase 0.1% formic acid and methanol (53:50, v/v) was used to determine the dicamba and the detector wavelength was set to 220 nm (Desipioa et al., 2019). The following chromatographic conditions were used for the enalapril assay method. The mobile phase contains a mixture of 0.02M NaH₂PO₄ buffer (pH 3.0 adjusted with H₃PO₄)

and acetonitrile in the ratio 95:5 (v/v) (Koppala et al., 2017). The analyses of the ibuprofen decay were carried out isocratically with a methanol/water (with 1% phosphoric acid) 68:32 (v/v) mixture as the mobile phase and detector wavelength was 228 nm (Loaiza-Ambuludi et al., 2013). The mobile phase for clomazone detection was methanol and water (65:35, v/v), adjusted to pH 4.0 with phosphoric acid and quantification was carried out with UV detection at 220 nm (Zanella et al., 2000). For the determination of loperamide the detector was set to 226 nm. Compound was eluted using an isocratic mobile phase consisting of 0.1% sodium-octansulphonate, 0.05% triethylamine, 0.1% ammonium hydroxide (buffer) in water:acetonitrile (45:55, v/v). The mobile phase was adjusted to pH 3.2 with phosphoric acid (Velinov et al., 2019).

Table S1. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of atenolol

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	40.114	40.114	40.114
	10.0	40.733	33.548	38.563
	100.0	45.514	46.584	37.541
	1 000.0	46.126	48.387	31.254
UV/persulfate	0	15.473	15.473	15.473
	10.0	16.579	10.014	13.192
	100.0	21.714	21.345	13.554
	1 000.0	22.031	21.945	10.672
Fenton	0	50.115	50.115	50.115
	10.0	/	/	48.374
	100.0	/	/	43.541
	1 000.0	/	/	40.051
photo-Fenton	0	56.735	56.735	56.735
	10.0	/	/	54.784
	100.0	/	/	50.053
	1 000.0	/	/	47.341
UV/TiO ₂	0	82.235	82.235	82.235
	10.0	82.907	75.033	80.571
	100.0	87.254	89.378	77.497
	1 000.0	88.001	91.545	70.369

Table S2. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of atrazine

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	39.619	39.619	39.619
	10.0	41.213	31.046	37.718
	100.0	44.578	46.832	35.491
	1 000.0	45.694	47.597	30.563
UV/persulfate	0	66.895	66.895	66.895
	10.0	67.548	60.064	64.677
	100.0	71.639	73.347	63.046
	1 000.0	72.056	75.218	56.421
Fenton	0	59.870	59.870	59.870
	10.0	/	/	56.012
	100.0	/	/	54.243
	1 000.0	/	/	50.377
photo-Fenton	0	100	100	100
	10.0	/	/	91.407
	100.0	/	/	87.153
	1 000.0	/	/	79.055
UV/TiO ₂	0	37.655	37.655	37.655
	10.0	38.975	30.043	36.045
	100.0	43.747	44.721	35.123
	1 000.0	44.098	46.798	29.348

Table S3. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of cyprodinil

Process	Concentration ion (mmol dm^{-3})	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/ H_2O_2	0	94.362	94.362	94.362
	10.0	100	87.049	89.391
	100.0	100	100	84.014
	1 000.0	100	100	77.553
UV/persulfate	0	10.846	10.846	10.846
	10.0	11.536	7.489	10.015
	100.0	17.792	17.345	8.632
	1 000.0	18.041	18.098	6.749
Fenton	0	67.763	67.763	67.763
	10.0	/	/	65.637
	100.0	/	/	64.326
	1 000.0	/	/	57.721
photo-Fenton	0	79.996	79.996	79.996
	10.0	/	/	77.341
	100.0	/	/	74.458
	1 000.0	/	/	67.364
UV/ TiO_2	0	92.606	92.606	92.606
	10.0	93.088	85.641	87.40
	100.0	97.397	98.377	82.17
	1 000.0	98.674	98.954	75.14

Table S4. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of dicamba

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	77.818	77.818	77.818
	10.0	79.541	70.749	76.431
	100.0	82.745	85.354	70.439
	1 000.0	83.639	87.092	65.728
UV/persulfate	0	5.349	5.349	5.349
	10.0	6.458	4.015	5.301
	100.0	6.941	12.466	5.587
	1 000.0	7.526	13.952	4.012
Fenton	0	54.977	54.977	54.977
	10.0	/	/	51.052
	100.0	/	/	50.437
	1 000.0	/	/	45.731
photo-Fenton	0	68.024	68.024	68.024
	10.0	/	/	66.347
	100.0	/	/	65.291
	1 000.0	/	/	87.458
UV/TiO ₂	0	83.811	83.811	83.811
	10.0	83.359	76.047	82.578
	100.0	88.264	90.569	78.421
	1 000.0	90.021	92.515	72.693

Table S5. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of enalapril

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	39.115	39.115	39.115
	10.0	40.075	32.043	38.346
	100.0	43.547	46.721	37.921
	1 000.0	45.034	48.798	32.395
UV/persulfate	0	15.473	15.473	15.473
	10.0	16.639	11.397	13.459
	100.0	22.594	22.658	13.365
	1 000.0	23.012	23.092	10.021
Fenton	0	57.115	57.115	57.115
	10.0	/	/	55.734
	100.0	/	/	50.526
	1 000.0	/	/	47.539
photo-Fenton	0	66.735	66.735	66.735
	10.0	/	/	64.327
	100.0	/	/	63.568
	1 000.0	/	/	56.441
UV/TiO ₂	0	69.646	69.646	69.646
	10.0	70.358	63.576	67.592
	100.0	74.647	76.482	64.371
	1 000.0	75.951	78.391	57.834

Table S6. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of ibuprofen

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	58.747	58.747	58.747
	10.0	59.384	51.675	56.347
	100.0	63.476	65.842	51.256
	1 000.0	64.291	67.361	49.418
UV/persulfate	0	48.769	48.769	48.769
	10.0	49.538	41.365	46.452
	100.0	54.247	55.879	41.376
	1 000.0	55.396	56.348	40.018
Fenton	0	77.452	77.452	77.452
	10.0	/	/	75.723
	100.0	/	/	74.458
	1 000.0	/	/	67.614
photo-Fenton	0	100	100	100
	10.0	/	/	100
	100.0	/	/	100
	1 000.0	/	/	100
UV/TiO ₂	0	48.747	48.747	48.747
	10.0	49.098	41.364	47.041
	100.0	55.027	55.217	46.695
	1 000.0	55.963	57.098	41.483

Table S7. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of clomazone

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	59.601	59.601	59.601
	10.0	60.381	52.731	57.347
	100.0	65.753	66.645	54.621
	1 000.0	66.642	68.286	51.519
UV/persulfate	0	38.587	38.587	38.587
	10.0	39.346	31.876	36.421
	100.0	45.721	45.019	34.798
	1 000.0	46.392	46.332	29.236
Fenton	0	58.611	58.611	58.611
	10.0	/	/	56.491
	100.0	/	/	53.015
	1 000.0	/	/	49.382
photo-Fenton	0	69.601	69.601	69.601
	10.0	/	/	65.313
	100.0	/	/	64.685
	1 000.0	/	/	57.291
UV/TiO ₂	0	79.167	79.167	79.167
	10.0	80.311	73.189	73.460
	100.0	84.465	86.356	72.319
	1 000.0	86.732	88.274	65.085

Table S8. Effect of HCO_3^- , CO_3^{2-} and Cl^- ions concentrations on the removal efficiency of loperamide

Process	Concentration ion (mmol dm ⁻³)	Decolorization (%)		
		HCO_3^-	CO_3^{2-}	Cl^-
UV/H ₂ O ₂	0	71.391	71.391	71.391
	10.0	72.391	65.189	67.491
	100.0	76.457	76.356	66.337
	1 000.0	77.926	88.274	59.981
UV/persulfate	0	58.278	58.278	58.278
	10.0	59.931	51.364	57.371
	100.0	64.275	65.279	53.956
	1 000.0	65.364	67.581	49.083
Fenton	0	81.391	81.391	81.391
	10.0	/	/	75.397
	100.0	/	/	74.451
	1 000.0	/	/	67.286
photo-Fenton	0	100	100	100
	10.0	/	/	100
	100.0	/	/	100
	1 000.0	/	/	100
UV/TiO ₂	0	82.166	82.166	82.166
	10.0	83.176	76.347	76.639
	100.0	87.394	89.981	74.351
	1 000.0	89.852	92.654	66.082

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