Supplementary Materials

Mechanistic Model and Optimization of the Diclofenac Degradation Kinetic for Ozonation Processes Intensification

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Content

S1. Six-Flux Model parameters

In Table S1 were presented the constants required to compute the LVRPA for a given point at the flotation cell based in equations (x-y). The scattering and absorption coefficients were taken for the Evonik p25.

Table S1. Constants employed to estimate the LVRPA.

Constants		Value	Units
Intensity	I_0	2.06×10^{-5}	$Einstein\ s^{-1}\ m^{-2}$
Scattering coefficient	σ	5420	$m^2\ kg^{-1}$
Absorption coefficient	κ	287	$m^2\ kg^{-1}$

First, the scattering albedo ω_{corr} was computed according to Equation (S1), then, by replacing within Equations (S2) and (S3), the corrected value for this variable was obtained (S4). Here p_s, p_b, and p_f were the sides, backward and forward scattering probabilities.

$$\omega = \frac{\sigma}{\kappa + \sigma} \tag{S1}$$

$$a = 1 - \omega p_f - \frac{4\omega^2 p_s^2}{1 - \omega p_f - \omega p_b - 2\omega p_s} \tag{S2}$$

$$b = \omega p_b + \frac{4\omega^2 p_s^2}{1 - \omega p_f - \omega p_b - 2\omega p_s} \tag{S3}$$

$$\omega_{corr} = \frac{b}{a} \tag{S4}$$

This value was used to calculate the corrected wavelength λ_{corr} and the optical thickness τ according to Equations (S5) and (S6). Then, the apparent value for the optical thickness τ_{app} was computed from (S7). Finally, the six-flux model parameter γ was obtained by equation (S8).

$$\lambda_{corr} = \frac{1}{a(\sigma - \kappa)C_{mp}\sqrt{1 - \omega_{corr}^2}} \tag{S5}$$

$$\tau = (\sigma + \kappa)C_{mp} r_p \tag{S6}$$

$$\tau_{app} = a\tau\sqrt{1 - \omega_{corr}^2} \tag{S7}$$

$$\gamma = \frac{1-\sqrt{1-\omega_{corr}^2}}{1+\sqrt{1-\omega_{corr}^2}}\exp(-2\tau_{app}) \quad \text{(S8)}$$

S2. Mass Transfer

The estimated values for the mass constants at the flotation cell were summarized in Table S2.

Table S2. Mass transfer constants for the flotation cell.

Constants	Value	Units
k_L	4.56×10^{-3}	$m\,min^{-1}$
a	220.33	m^{-1}
$\phi_{(g)}$	4.13×10^{-3}	---
d_b	0.11	mm
D_{O_3}	7.80×10^{-8}	$m^2\,min^{-1}$

S3. Kinetic Regime

Figures S1–S3 depicted the estimated values of the Hatta number based on a first-order rate law for the ozonation, catalytic ozonation, and photocatalytic ozonation processes.

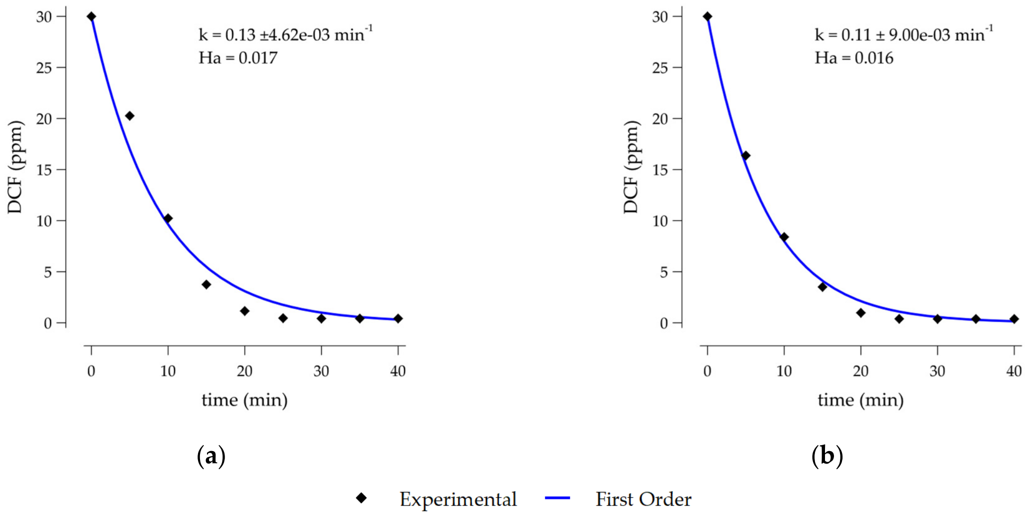


Figure S1. First-order rate law predictions for the diclofenac concentration in the ozonation process at (**a**) 2.66 and (**b**) 7.44 ppm in the ozone dose.

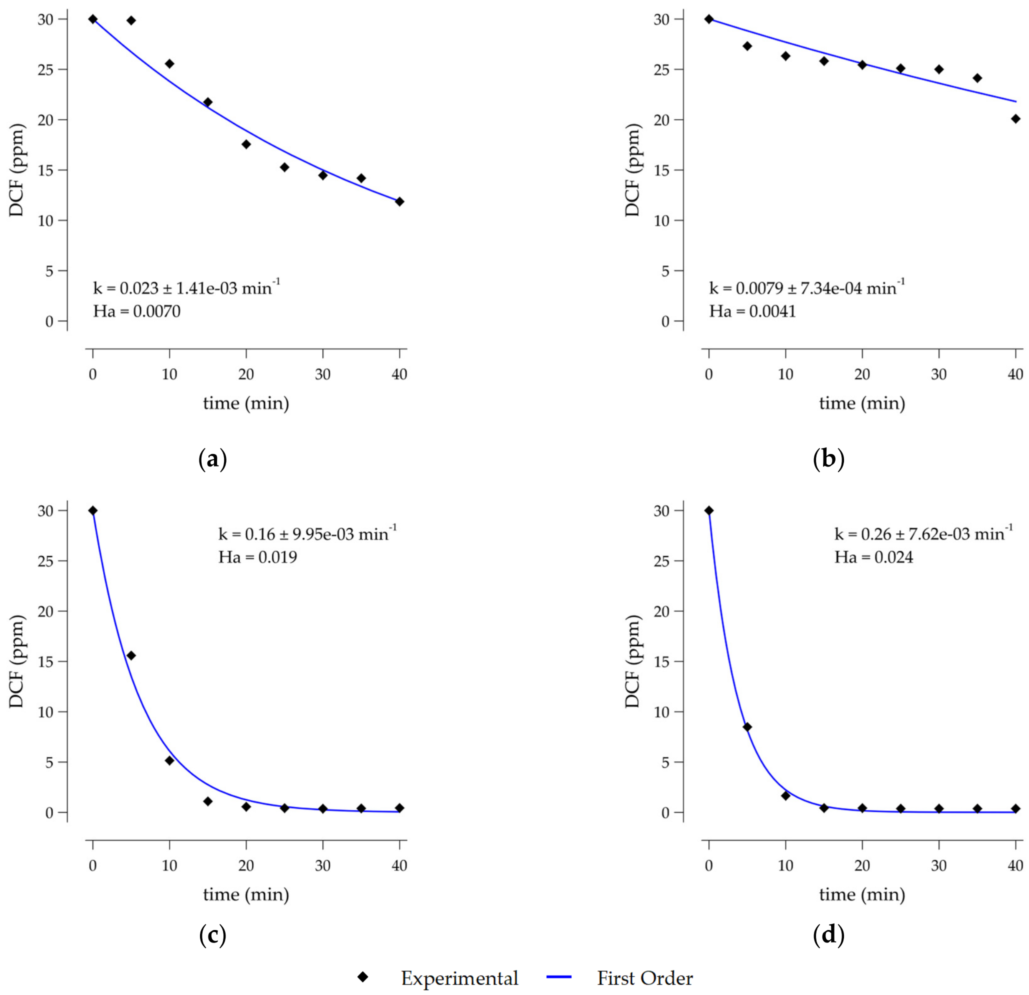
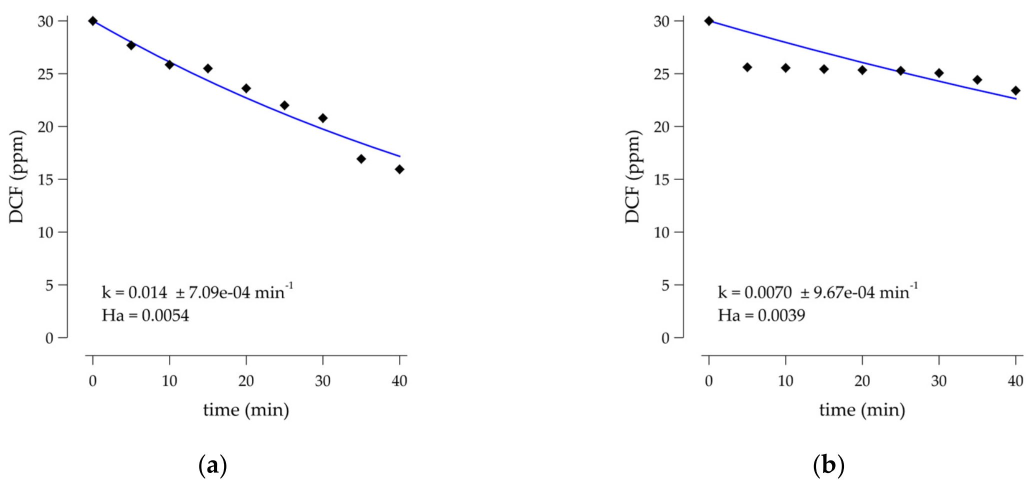


Figure S2. First-order rate law predictions for the diclofenac concentration in the catalytic ozonation process at (**a**) 2.66 & 300, (**b**) 2.66 & 800, (**c**) 7.40 & 300, (**d**) 7.40 & 800 ppm in the ozone dose and the catalyst load respectively.



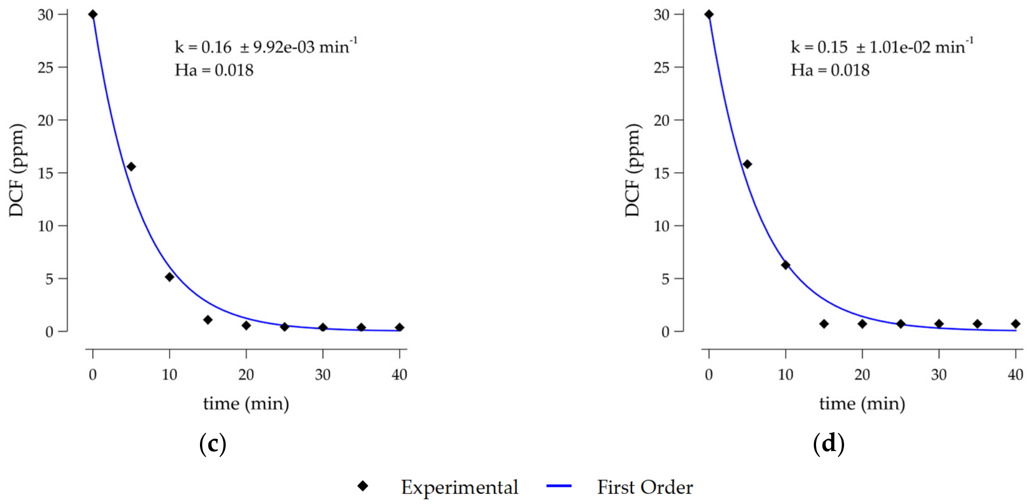


Figure S3. First-order rate law predictions for the diclofenac concentration in the photocatalytic ozonation process at (**a**) 2.66 & 300, (**b**) 2.66 & 800, (**c**) 7.40 & 300, (**d**) 7.40 & 800 ppm in the ozone dose and the catalyst load respectively.

S4. Electrical Energy per Order

Table S3. Electrical energy per order (EE/O) for each process conditions.

Process	Ozone dose (ppm)	Catalyst load (ppm)	EE/O ($kWh\ m^{-3}$)
Ozonation	2.66	---	14.44
	7.40	---	17.07
Catalytic Ozonation	2.66	300	81.62
	2.66	800	237.64
	7.40	300	11.73
	7.40	800	7.22
Photocatalytic Ozonation	2.66	300	158.47
	2.66	800	316.45
	7.40	300	13.86
	7.40	800	14.79