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# Trace Organic Compound Removal from Wastewater Reverse-Osmosis Concentrate by Advanced Oxidation Processes with UV/$O_3$/$H_2O_2$

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**Equation S1.** – Determination protocol of the scavenging rate $K_{SC}$.

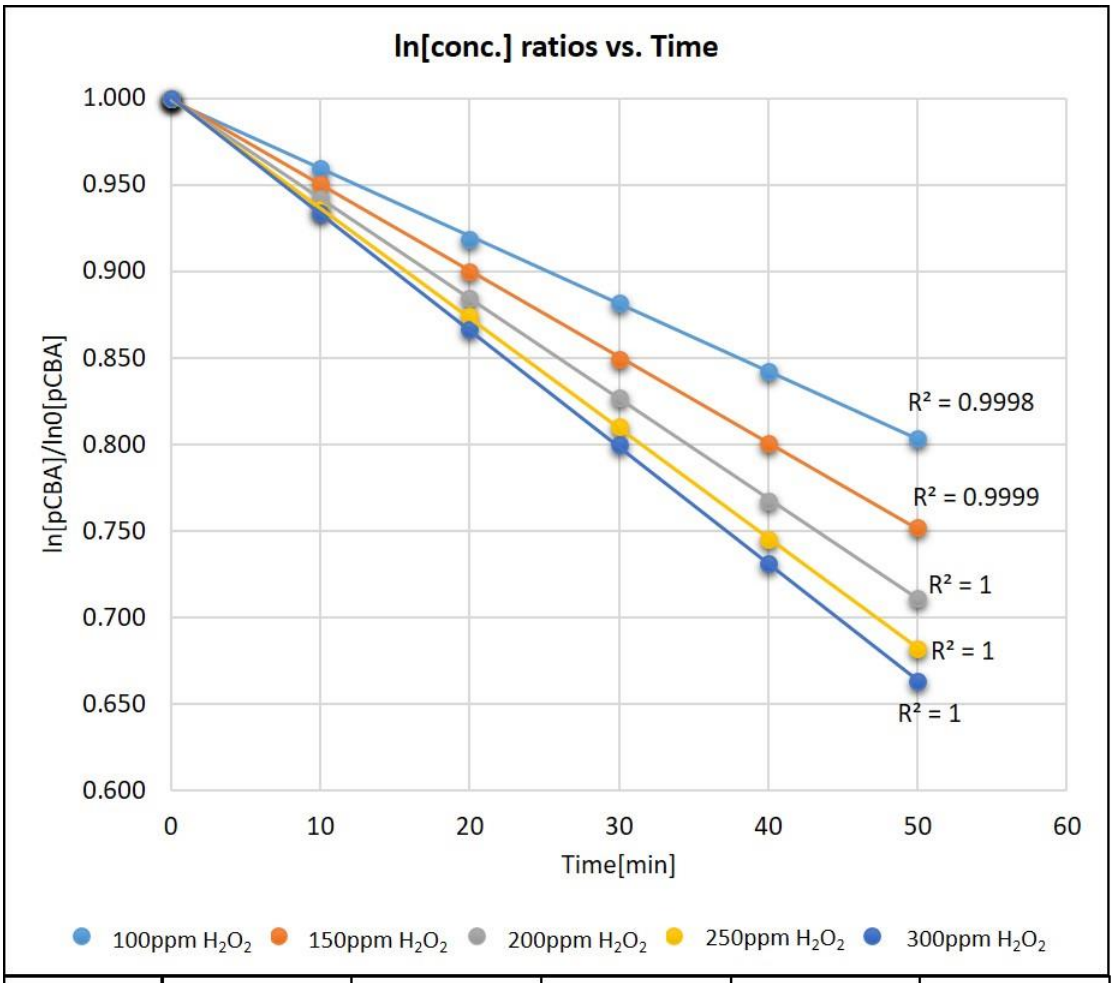
Pseudo-first order degradation rate constant of para-chlorobenzoic acid (pCBA) at the steady state concentration of OH·, In the case of low pCBA concentration, where its contribution to the total scavenging is negligible:

$$\frac{R^{form}}{K'} = A = \pi r^2 \frac{K_{SC}}{K_{OH,pCBA}} + \frac{K_{OH,H2O2}[H2O2]}{K_{OH,pCBA}} \quad (S1)$$

$K_{SC}$ - scavenging rate of the water matrix [1/s]; $R^{form}$ - Rate of formation for the OH· under the specific conditions and it is depending on the Ultraviolet (UV) lamp intensity and on the hydrogen peroxide added concentration [$H_2O_2$]; $K_{OH,H2O2}$, $K_{OH,pCBA}$ - Second-order rate constants $H_2O_2$ and pCBA, respectively, with OH·, where $K_{OH,pCBA} = 5 \times 10^9$ M $S^{-1}$.; K' - slope obtained for the log transformation of pCBA concentrations, from each set of UV applied with different $H_2O_2$ concentrations.

UV/$H_2O_2$ degradation of pCBA was examined at different $H_2O_2$ concentrations, and the results were used to plot [$H_2O_2$] vs. $\frac{R^{form}}{K'}$. In other words, the equation could be describe as a linear regression, y=ax + b, where **y** is $\frac{R^{form}}{K'}$, **x** is the hydrogen peroxide concentration [$H_2O_2$], **a** (slope) is $\frac{K_{OH,H2O2}}{K_{OH,pCBA}}$ and **b** (intercept) is $\frac{K_{SC}}{K_{OH,pCBA}}$.

$K_{SC}$ could be calculated by extracting the intercept (b) from the linear regression equation.




| | 100ppm H2O2 | 150ppm H2O2 | 200ppm H2O2 | 250ppm H2O2 | 300ppm H2O2 |
|---|---|---|---|---|---|
| Slope=K' | -0.003925 | -0.004977 | -0.005785 | -0.006363 | -0.006746 |
| Abs K' | 0.003925 | 0.004977 | 0.005785 | 0.006363 | 0.006746 |

**Figure S1.** -K' calculations.

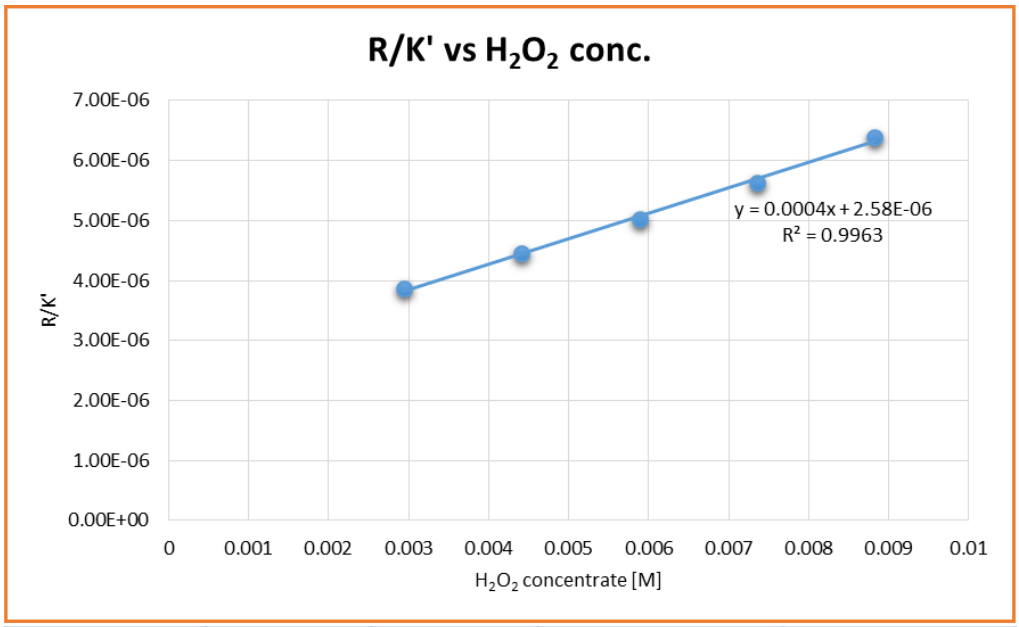
**Equation S2.** - $R^{form}$ calculations protocol.

$$R^{form} = \sum_{200-300} \frac{10^{-3} \times E_p^0(\lambda)\varepsilon(\lambda)\left[1-10^{-a(\lambda)z}\right]}{a(\lambda)z} \times \varphi \times [H_2O_2] \quad \text{(S2)}$$

$E^0_p$ – incident photon irradiance (Es $cm^{-1}$ $s^{-1}$); ε(λ) - fraction of UV energy absorbed by $H_2O_2$ at each wavelength ($M^{-1}$ $cm^{-1}$); a(λ) - solution absorption coefficient ($cm^{-1}$); z – depth of solution (cm); $\varphi$ – quantum yield of OH· by $H_2O_2$ UV photolysis (mol $Es^{-1}$);

**Table 1.** - $R^{form}$ calculations based on UV measurements of the different $H_2O_2$ concentrations in the WWROC samples after UV radiation.

| $H_2O_2$[ppm] | $H_2O_2$ [M] | $R^{form}$ |
|---|---|---|
| 100 | $2.94 \times 10^{-3}$ | $1.52 \times 10^{-8}$ |
| 150 | $4.41 \times 10^{-3}$ | $2.22 \times 10^{-8}$ |
| 200 | $5.88 \times 10^{-3}$ | $2.91 \times 10^{-8}$ |
| 250 | $7.35 \times 10^{-3}$ | $3.58 \times 10^{-8}$ |
| 300 | $8.82 \times 10^{-3}$ | $4.32 \times 10^{-8}$ |




| $H_2O_2$ [ppm] | $H_2O_2$[M] | (K') | $R^{form}$ | R/K' |
|---|---|---|---|---|
| 100 | 2.94E-03 | 3.93E-03 | 1.52E-08 | 3.87E-06 |
| 150 | 4.41E-03 | 4.98E-03 | 2.22E-08 | 4.45E-06 |
| 200 | 5.88E-03 | 5.79E-03 | 2.91E-08 | 5.03E-06 |
| 250 | 7.35E-03 | 6.36E-03 | 3.58E-08 | 5.63E-06 |
| 300 | 8.82E-03 | 6.75E-03 | 4.32E-08 | 6.40E-06 |

Figure S2. –plotting $\frac{R^{form}}{K'}$ as a function of the [$H_2O_2$]. The derived linear equation intercept is multiplied by $K_{OH,pCBA}$=5 × $10^9$ $M^{-1}$ $S^{-1}$ to calculate the scavenging rate $K_{SC}$.

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