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PARAMETER ESTIMATION BY BAYESIAN STATISTICS OF KINETIC MODELS IN OZONATION PROCESSES

Júlia Toffoli de Oliveira
Liliana Amaral Féris
Federal University of Rio Grande do Sul – Department of Chemical Engineering. Ramiro Barcelos Street, 2777. Porto Alegre – RS, Postcode 90035-007 - Brazil.
juliatdo@gmail.com, liliana.feris@gmail.com.

Diego Cardoso Estumano
Federal University of Pará – Faculty of Biotechnology. Augusto Corrêa Street, 01. Belém – PA, Postcode 66075-110 – Brazil.
dcestumano@ufpa.br

Abstract. *Ozonation is an advanced oxidative process that has been studied by researchers to improve water and wastewater treatments. Advanced oxidative processes (AOPs) are based on the generation of the hydroxyl radical (·OH), which is a powerful oxidizing agent, being able to degrade or even mineralize the toxic and persistent components that are not removed during the conventional processes. The kinetic models of ozonation, in which the most used is the pseudo-first order model, provide important information about the process, such as: through which oxidation route is mostly like to occur, which is informed through the parameters present in the models ($k_{O3,P}$ and $k_{OH,P}$) and by a parameter called exposure ratio (Rt). This work aims to evaluate the kinetic constants of the reactions involving ozone, with data from the literature, in order to facilitate and guide the study of the technique in different pollutants for posteriors works. For the estimation of the parameters, Bayesian statistics was applied, by the method of Monte Carlo Markov Chain (MCMC) through the Metropolis-Hastings algorithm. The results obtained in this work were adequate and satisfactory. Also, through this work it is possible to observe that using the exposure ratio for the kinetic models directly interferes in the parameter values and that the MCMC method is an efficient and reliable mathematical approach.*

Keywords: *ozonation, kinetics, simulation, parameter estimation, Bayesian statistics*.

1. INTRODUCTION

Advanced oxidative processes (AOPs) have been gaining space in academic research due to the increase in the complexity of the effluents that are being generated nowadays, therefore, it needs to be previously treated before being released into the water bodies. Among them, ozonation is being widely used for the disinfection of wastewater, but also as a possible treatment for the oxidation of emerging and recalcitrant pollutants present in effluents, being able to increase its biodegradability, on account of being a fast and easy-to-operate process (Lara-ramos et al., 2021; Olsińska, 2019). However, the method has limitations such as the cost of operation involved, being its main disadvantage, and problems of mass transfer due to the solubility of ozone in water, therefore, the design of the reactor in which it will be used for the process of ozonation is essential, thus, the kinetics involving this technology are extremely important to evaluate the efficiency and mechanism of the process as well as to design the reactor (Gomes *et al.*, 2017; Gunten, 2018).

In addition, it is important to highlight that the pH of the solution directly affects the oxidation of the compounds by the ozonation process. The oxidation can occur in two ways, via direct oxidation, by molecular ozone (O_3 – 2,07 V), occurring predominantly in acidic medium which has a selective reactivity toward organic pollutants; or indirectly, through oxidation by hydroxyl radicals (·OH – 2,8V) generated during the process, generally in a basic medium which is a non-selective oxidant and highly reactive; on the other hand, in neutral pH solutions, ozonation can occur by both oxidation routes simultaneously (Elovitz & Gunten, 1999; Benbelkacem et al., 2010). Although both oxidants are effective in organic compounds the ·OH reacts with certain O_3-resistant pollutants, therefore its formation is preferable (Gunten & Sonntag, 2020).

To predict the efficiency of the removal of pollutants, the determination of ·OH and O_3 concentrations are necessary, in which it is possible through the parameters present in the ozonation kinetics models, characterized as an inverse problem. The kinetics of ozone reaction is commonly described as pseudo-first-order reaction (Elovitz & Gunten, 1999; Pandiselvam *et al.*, 2015; Gomes *et al.*, 2017; Guo *et al.*, 2018; Gunten & Sonntag, 2020). Thus, the effectiveness of the oxidation processes depends on two factors: the rate of reaction of the target compounds with ozone and the rate of ozone consumption by water matrix (Gardoni *et al.*, 2012). To determine the parameters a Bayesian technique was applied, the Markov Chain Monte Carlo (MCMC) method regarding the Metropolis-Hastings acceptation/rejection algorithm.

Therefore, the aim of this work is to apply a method, through a computational resource, to predict the kinetic parameters during the ozonation process using experimental data from the literature, in this case the ozonation of caffeine by Souza (2016), which will be used as a probability distribution a priori for the MCMC. The procedure developed in this work, to estimate the kinetic parameters, will facilitate future works on the ozonation of pollutants present in the residual waters.

2. DIRECT MODELS OF OZONATION

For ozonation, kinetic models and their reaction rate constants for several organic compounds are identified and described in the literature to better understand the mechanisms that involve the ozonation process during the reaction. There are several methods to determine the ozone rate constants with a given compound, the most reliable one and the least applied is the direct method, which will be used in the present work. They are more reliable because there is an uncertainty involved in in the most common method that uses competition kinetics, therefore, causing a greater error in the estimation of the rate constants, however the direct model is more difficult to calculate since they need mathematical resources for its resolution (Hoigné & Bader, 1983; Gunten & Sonntag, 2020). Thus, the Markov Chain Monte Carlo method was applied. The kinetic models used in the present work are described in item 2.1.

2.1 Ozone kinetic

The mechanism of oxidation of a generic compound (P) by ozonation is (Gunten, 2003):

$$P + O_3 \rightarrow \text{products}$$

The kinetics of ozone with organic compounds is typically a pseudo-first order model, according to Equation (1) (Gunten, 2003).

$$d[P]/dt = k[P][O_3] \tag{1}$$

where, k is the kinetic constant of pseudo-first order model ($M^{-1}.s^{-1}$) for the ozonation process; P is the concentration of the compound of interest (M^{-1}); O_3 is the concentration of ozone (M^{-1}).

However, the oxidation of compounds is characterized by the action of two oxidants, ozone (O_3) and hydroxyl radicals (·OH), thus, the kinetic can be described according to Equation (2) (Gunten, 2003).

$$-d[P]/dt = k_{o_{3,P}}[P][O_3] + k_{OH,P}[P][OH] \tag{2}$$

where, $k_{o_{3,P}}$ and $k_{OH,P}$ are the are the kinetic constants for the compound of interest P ($M^{-1}.s^{-1}$) for the oxidation via O_3 and via ·OH, respectively; OH is the concentration of hydroxyl radicals (M^{-1}). To obtain the concentration of ·OH usually it is applied the competition method, which was used by Souza (2016), however it is an indirect measure causing a greater error in the estimation of the parameters (Gunten & Sonntag, 2020).

To improve the model, Elovitz & Gunten (1999), proposed a new term, the ratio of ·OH exposure to O_3 exposure defined by R_t, according to Equation (3).

$$R_t = \int [OH]\, dt \,/\, \int [O_3]\, dt \tag{3}$$

The R_t term is used to predict the removal of organic pollutants since the concentration of ·OH during the reaction is unknown, therefore, it can be removed from the kinetic model. It is important to highlight that the R_t is directly affected by: the initial dose of O_3; concentration and composition of the pollutant; temperature and pH of the solution; however, is reported in the literature that R_t is typically in the range of 10^{-7}–10^{-9} (M/M) for various waters with different quality parameters such as pH, alkalinity, concentration of dissolved organic carbon and temperature. The lower range of R_t value (10^{-9}) represent typical conditions for the secondary phase of ozonation (after 100 s) and the upper range (10^{-7}) is

observed during the initial phase (before 100 s) or throughout a combination of POAs (Elovitz *et al*., 2000; Yong & Lin, 2013; Kwon *et al.*, 2017). Substitution of Equation (3) into Equation (2) results in Equation (4).

$$-d[P]/dt = \left(k_{o_{3,P}} + k_{OH,P}\, R_t\right)[P] \int [O_3]\, dt \tag{4}$$

Therefore, the values of R_t found in the literature will be used in the present work as a priori information along with the values of the kinetic parameters found for the ozonation of caffeine by Souza (2016), which is $k_{o_{3,P}}$= 697.46 $M^{-1}.s^{-1}$ and $k_{OH,P}$= 6.41.10^9 $M^{-1}.s^{-1}$, where P is caffeine. The initial concentration used for the experiments of the pollutant was 1 $g.L^{-1}$, with an ozone flow of 10 $mL.min^{-1}$ and the time of the ozonation process was 30 min.

The fraction of $\int [OH]$ can be calculated as Equation (5) (Gunten, 2003).

$$\int [OH] = \left(k_{OH,P}\, R_t\right) / \left(k_{o_{3,P}} + k_{OH,P}\, R_t\right) \tag{5}$$

3. BAYES THEOREM

A Bayesian approach was used to estimate de parameters ($\boldsymbol{\theta}$) of the direct models of ozonation. This method essentially consists of using all the information available to in order to reduce uncertainty in inference or decision-making problems, relating a statistical analysis of a density a posteriori probability ($p(\boldsymbol{\theta}|\boldsymbol{X})$), which is the conditional probability of the parameters given the measures; with the likelihood ($p(\boldsymbol{X}|\boldsymbol{\theta})$), which is the conditional probability of the measures given the a priori parameters. However, the posterior probability distribution cannot be calculated directly, for this the Monte Carlo Markov Chain method implemented by the Metropolis-Hastings algorithm was applied (Naveira-Cotta, 2009; Orlande *et al.*, 2011; Wang *et al.*, 2019; Amador *et al.*, 2021).

The posterior probability density function can be written as Equation (7), as being proportional to the product of the likelihood and a priori distribution; and the likelihood function is formulated as Equation (8), assuming that the errors are normally distributed, independent and homoscedastic.

$$p(\boldsymbol{\theta}|\boldsymbol{X}) \propto p(\boldsymbol{X}|\boldsymbol{\theta})\, p(\boldsymbol{\theta}) \tag{7}$$

$$p(\boldsymbol{X}|\boldsymbol{\theta}) = \frac{1}{(2\pi\sigma_T^2)^{\frac{-n}{2}}} \exp\left(-\frac{(X - F(\boldsymbol{\theta}))^T\, (X - F(\boldsymbol{\theta}))}{2\sigma_T^2}\right) \tag{8}$$

where, $p(\boldsymbol{\theta}|\boldsymbol{X})$ is the probability distribution density function $\boldsymbol{\theta}$ given $\boldsymbol{X}$ a posteriori observations; $\boldsymbol{X}$ is the data vector; $\boldsymbol{\theta}$ is the vector of the parameters of interest; $p(\boldsymbol{X}|\boldsymbol{\theta})$ is the likelihood; $p(\boldsymbol{\theta})$ is the a priori distribution of the parameters; σ_T^2 is the variance of the measurement uncertainty and $\boldsymbol{F}$ is the data calculated as a function of the parameters to be estimated.

4. MONTE CARLO VIA MARKOV CHAIN METHOD

To obtain the approximation of the probability distribution density function was used the Monte Carlo Markov Chain method. The MCMC is an interactive tool, based on the Markov chains and which aims to obtain a sample of the posterior distribution and calculate sample estimates of characteristics of the distribution that is under study (Spall, 2003; Orlande *et al.*, 2011). The MH algorithm was developed by Metropolis *et al.* (1953) and Hastings (1970) and updates the state of the Markov chain (Spall, 2003; Craiu & Rosenthal, 2014). The algorithm is based on the reject and accept method, in which a candidate value (θ*) is generated from an auxiliary distribution and accepted with a given probability guaranteeing the convergence of the chain for the equilibrium distribution. The MH algorithm is based in the following steps (Metropolis *et al.*, 1953; Hastings, 1970; Tozzo-Martins & Silva, 2007; Orlande *et al.*, 2011).

1. Choose the number n of states (number of simulations);
2. Initialize the interaction counter i=0 and specify an initial value (θ^0);
3. A candidate value q(θ*) is generated from the distribution q(θ*|θ) as shown in Equation (9):

$$\theta^* = \theta(1 + w\varepsilon) \tag{9}$$

where, w is the search step and ε is the random number of a uniform distribution U (0,1).

4. Calculate the acceptance probability α (θ, θ*) given by the Hastings Ratio, represented by Equation (10);

$$\alpha(\theta,\theta^*) = \min\left[1, \frac{p(\theta^*|X)\ q(\theta^*|\theta)}{p(\theta|X)\ q(\theta|\theta^*)}\right] \quad (10)$$

5. Generate a uniformly distributed auxiliary random sample: u ~ U (0,1);
6. If u ≤ α (θ, θ*) the new value is accepted and θ(i+1) = θ* is accepted, otherwise θ* is rejected and θ(i+1) = θ (i);
7. Increment the counter from i to i+1 and go back to step 3 until i=n.

5. RESULTS AND DISCUSSIONS

As mentioned before, the present study will consider the estimation of two parameters, $k_{O_{3,P}}$ and $k_{OH,P}$, for the process of caffeine ozonation by Souza (2016). Figure 1 shows the ratio of concentration of the compound P, in this case caffeine, over time.

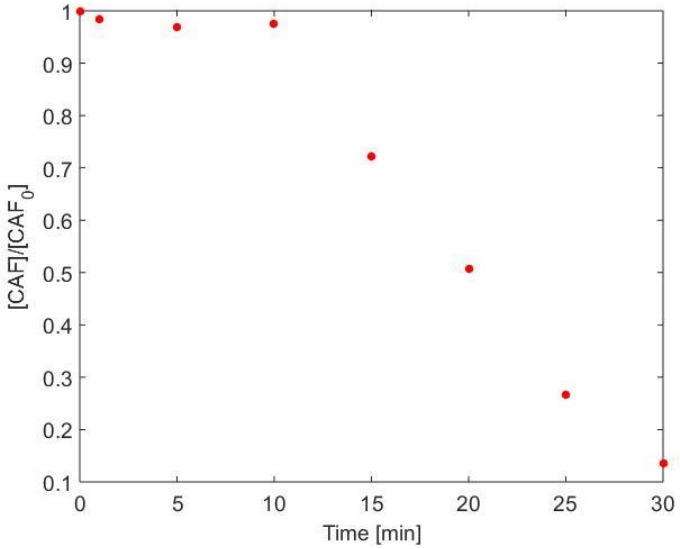

Figure 1. Ratio of concentration of caffeine over time for the ozonation process.
Available from: Souza (2016).

Two classical statistical metrics will be used to evaluate the accuracy of the results: the coefficient of determination (R^2) and the adjusted coefficient of determination (R^2_{ajstd}), which are widely known. The input data used for the Markov Chain Monte Carlo method are shown in Table 1.

Table 1. Input data for the MCMC method.

n	Number of states in the Markov Chains	5000
w	Search step	0.003
C.I.	Credible interval	99%
σ_{med}	Standard-deviations for the likelihood function	[0.01, 0.02 and 0.05] max$((P/P_0)^{exp})$
θ^0	Initial estimation values of the parameters	[697.46 $M^{-1}.s^{-1}$ 6.41.10^9 $M^{-1}.s^{-1}$]

The initial estimates for all parameters were the values obtained by Souza (2016) and the previous information for each parameter was taken as a uniform distribution, with the lower interval equal to zero, and the superior interval equals to 10^4 times the parameter value. In addition, it is important to highlight that, as shown in Tab. 1, three different standard deviations were considered for the measurements: 1%, 2% and 5% of max $((P/P_0)^{exp})$. The choice of these deviations is due to the fact that obtaining the experimental data requires careful and precise analysis, since is a sensitive method. The measurements obtained by the method applied in the kinetic ozonation experiments is accurate to ±1%, in precise laboratories under controlled conditions, and in practical applications the accuracy has been shown to be within ±2% due to operating conditions that are not easily controlled, therefore, the deviations selected for the present study were 1%, 2% and 5% in order to observe the impact it has on the resolution of the method (Rakness *et al.*, 1996a; Rakness *et al.*, 1996b).

From the analysis of Fig. 2, it is possible to verify that the parameter $k_{O_{3,P}}$ converge after approximately 2500 states in the Markov Chain for σ_{med}= 0.01 and σ_{med}= 0.02, while for σ_{med}= 0.05 it takes more states to achieve the

convergence, showing that the kinetic models are very sensitive to high standard deviations. On the other hand, the parameter $k_{OH,P}$ has a difficult convergence illustrating the complexity of estimating this parameter, suggesting that the parameter $k_{OH,P}$ has low sensitivity (the sensitivity analyses about the parameters should be done), however the Markov chains for these cases are around an average value, even though they did not converge, an adequate fit was obtained. Nevertheless, for typical values of standard deviation found in the literature (1% and 2%), the parameters have a good convergence.

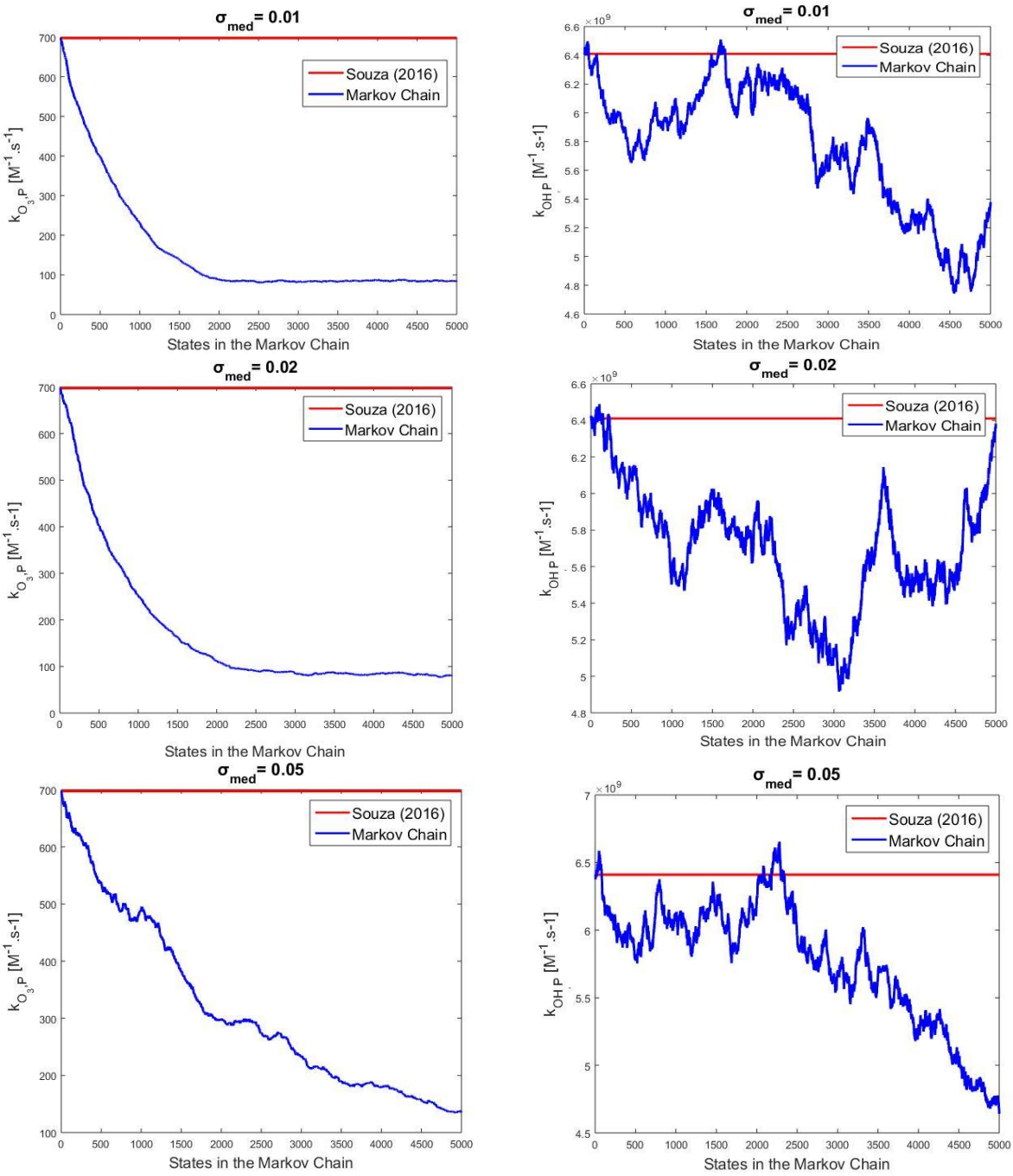

Figure 2. Comparison between the estimated concentrations, considering the three different standard deviations for the measurements, with the experimental data.

Table 2 shows the estimated parameters for each standard deviation of the measures considered and their respective metrics while the Fig. 3 illustrate the estimated and the experimental ratio of the compound P concentration curves with a credibility interval (C.I) of 99%.

Table 2. Comparison between the experimental and estimated parameters.

Standard deviation of the measurements	Parameter ($M^{-1}.s^{-1}$)	Experimental ($M^{-1}.s^{-1}$)	Estimated ($M^{-1}.s^{-1}$)	Metrics
σ_{med}= 0.010	$k_{o_{3,P}}$	697.46	84.69 (81.83 – 87.71)	R^2= 0.9917
	$k_{OH,P}$	6.41x10^9	5.33x10^9 (4.77x10^9 – 5.94x10^9)	R^2_{ajstd}= 0.9883
σ_{med}= 0.020	$k_{o_{3,P}}$	697.46	83.58 (77.22 – 87.98)	R^2= 0.9916
	$k_{OH,P}$	6.41x10^9	5.61x10^9 (4.94x10^9 – 6.34x10^9)	R^2_{ajstd}= 0.9883
σ_{med}= 0.050	$k_{o_{3,P}}$	697.46	176.89 (135.01 – 232.25)	R^2= 0.8599
	$k_{OH,P}$	6.41x10^9	5.32x10^9 (4.70x10^9 – 5.99x10^9)	R^2_{ajstd}= 0.8038

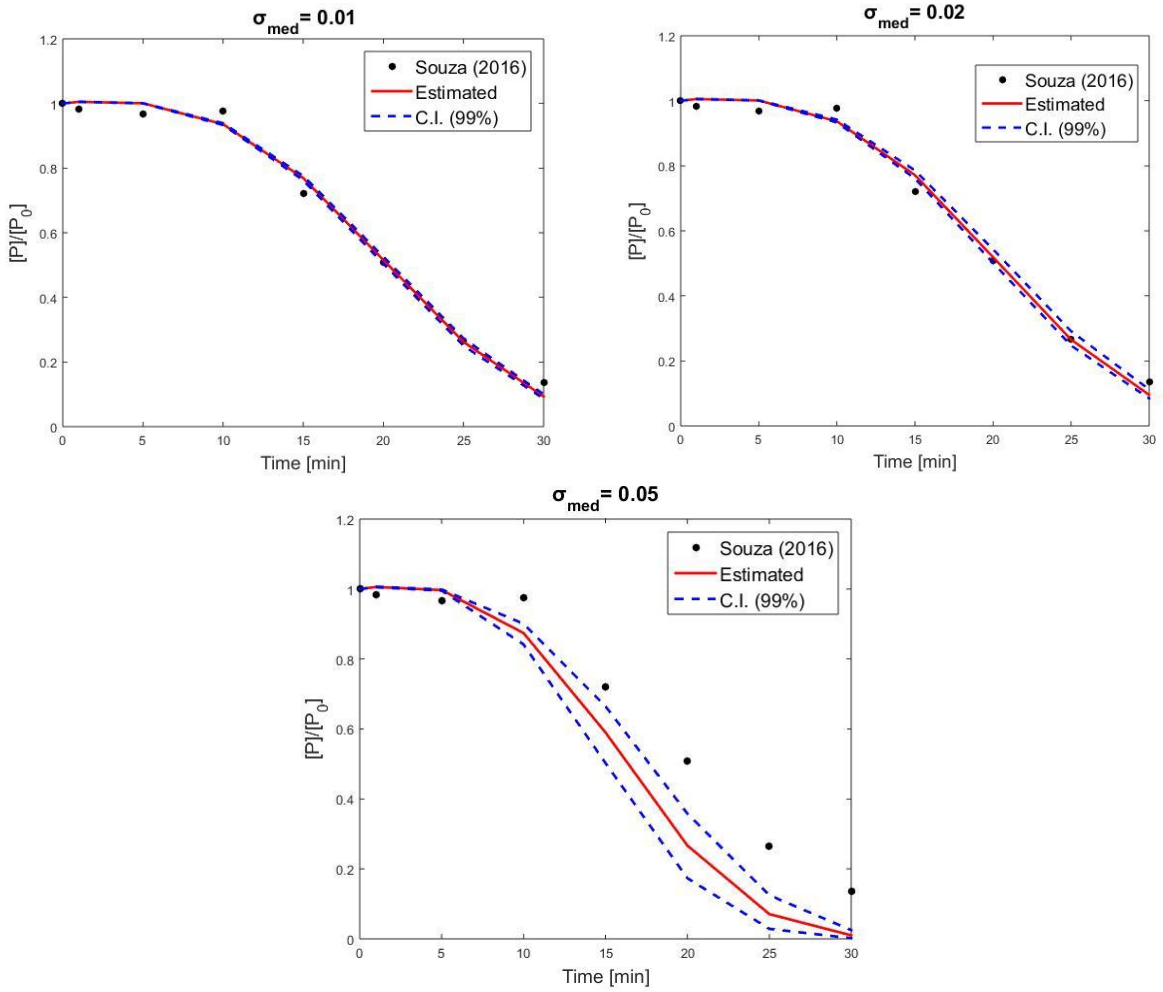

Figure 3. Comparison between the estimated concentrations, considering the three different standard deviations for the measurements, with the experimental data.

As expected, the largest deviation presented the worst results because it is a very sensitive experimental method, therefore, the greater the deviation, the worse the fit. On the other hand, for the deviations of 1% and 2%, the results were very similar and both obtained an adequate adjustment, showing a good correlation between the estimated values and those obtained experimentally by Souza (2016).

However, we can notice that there is a difference between the parameters estimated by MCMC and those obtained by the author by linear regression, even though they are in the same order of magnitude, the difference in the results can be explained by: the use of the exposure ratio term (R_t) to calculate the parameters, in which is not implemented by the author since the competition method was applied; and by the mathematical method itself, in which Bayesian Statistics was used instead of the Classical Statistics applied by Souza (2016). The ratio of exposure and the MCMC method, aim to reduce the uncertainty of the indirect model resulting in more reliable and accurate parameters. Therefore, it is possible to infer that these approaches are able to estimate the parameters and predict the concentration of the pollutant.

6. CONCLUSIONS

Through this study, using the exposure ratio term and the Markov Chain Monte Carlo Method via Metropolis-Hastings algorithm to obtain the parameters, it is possible to conclude that both approaches are accurate and promising for the estimation of the kinetic parameters of the ozonation models. These results were obtained using a uniform a priori distributions with the means equal to the exact values of the parameters, where different standard deviations were considered for the measurements.

The pollutant P concentration curves were very well estimated, even in the presence of noise in the measurements, showing a good potential for applying the method. From the results of the parameters, it is possible to observe the influence that the exposure ratio (R_t) and the standard deviations (σ_{med}) have in the estimation of the parameters. The authors intend to continue this study using the mathematical resource created in this work in other pollutants and for other kinetic models, with experimental measurements, in order to deepen and understand the mechanisms involved during the ozonation process.

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