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Application of Approximate Bayesian Computational for Estimate Parameter and Selection Model in Dynamic of HIV

Aplicação de Aproximação Bayesiana Computacional para Estimativa de Parâmetros e Seleção de Modelo in Dinâmica de HIV

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RESUMO

A aplicação de técnicas Bayesianas tem se tronado comum em bioengenharia, é comum realizar inferências sobre parâmetros e variáveis de estado que não podem ser mensurados. Este trabalho tem como objetivo aplicar a técnica de Aproximação Bayesiana Computacional para estimar parâmetros e selecionar modelos simultaneamente nos modelos que descreve a dinâmica de células importantes que representam o HIV. Três diferentes modelos dinâmicos foram usados para avaliar a verificação do algoritmo, esta verificação foi realizada com medidas simuladas. A técnica foi verificada e se mostrou ser robusta o suficiente para estimar parâmetros e selecionar o melhor modelo simultaneamente e por isso, esta se mostra ser uma técnica promissora.

Palavras-chave: técnica bayesiana; Aproximação Bayesiana Computacional; HIV

ABSTRACT

The application of Bayesian techniques is becoming common in bioengineering, as it is common to infer inferences about parameters and state variables that cannot be measured. This work aims to apply the Approximate Bayesian Computational technique to estimate parameters and select models simultaneously in models that describe the dynamic of important cells representing the HIV disease. Three different dynamic models were used to perform the algorithm's verification since the technique was used regarding synthetic measures. It was verified that the technique is robust enough to estimate and select the models studied simultaneously and this way showed be a promise technique for this objective.

Keywords: Bayesian technique; Approximate Bayesian Computational; HIV.

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INTRODUCTION

Acquired Immunodeficiency Syndrome (AIDS) is characterized by profound immunodeficiency, leading to opportunistic infections, secondary neoplasms, and neurological manifestations (Patil, 2014; Valerio et al, 2021). Although this syndrome has been the subject of research for a long time, much remains to be discovered. The difficulty of understanding the syndrome causes research to become multidisciplinary due several technologies must be developed to understand many processes related to dynamic of HIV. In a particular characteristic in this field is similar in many issues present in engineering research, which are the acknowledgment of parameters for to solve the mathematical formulations. In engineering is common use the classical statistics to determine the parameters, and the technique widely used is Least-Square. Other field from statistics that is becoming common apply to estimate parameters is the Bayesian Statistics, as well as the classical statistics several issues from the engineering was solved by techniques from Bayesian Statistics as can see example of such application in a adsorption, combustion, neurology, mass transfer, heat transfer.

In the classical statistics, several research types focus on the methodology for the solution of formulations of HIV dynamics and parameter estimates (Perelson, Kirscchner, De Boer, 1993; Wu, Ding, De Gruttola, 1998; Perelson and Nelson, 1999; Putter et al., 2002; Xia, 2003; Adams et al., 2007; Srivastava, Awasthi, Kumar, 2014). However, the application of the Approximate Bayesian Computational (ABC) has not yet been explored. This algorithm has the characteristic of estimating parameters and selecting models simultaneously. Such estimates are important due to selecting the best model, which has the consequence of determining which is the best hypothesis to describe the experimental data. Besides, the estimation of the parameters allows inferences to be made as to which measures cannot be obtained directly (Toni et al., 2009; Toni and Stumpf, 2009; Toni and Stumpf, 2010; Santos et al., 2020a; Santos et al., 2020b).

Therefore, this work aims to evaluate the application of the ABC technique through the use of 3 different models that describe the cell dynamics that characterize the HIV syndrome previously described by Perelson and Nelson (Perelson and Nelson, 1999) and Perelson et al. (Perelson, Kirscchner, De Boer, 1993). These models are based on different hypothesis. The procedure of estimate parameters and select the model is interesting to identify the main phenomenon involved through mathematical modeling

and estimating information that are not measured. In this work, to evaluate the application of Approximate Bayesian Computational in these models were used simulated regarding uncertainties as normal distribution, uncorrelated and independent. Besides the novelty of apply the ABC technique in dynamic of HIV models, in this work was evaluated a strategy to determine the tolerance for each population based on the previous particles accepted in the previous population, this way optimizing the algorithm, once the present in the literature is necessary define the quantity of population and the tolerance in each population.

2. HIV DYNAMIC MODELS

Models that represent the dynamics of HIV are commonly found in the literature and for different scenarios. In this work, we chose to use 3 similar models that present as populations variables of uninfected $CD4^+$ T cells (T), latently infected $CD4^+$ T cells (T*), productively infected cells (T**), and free virus (V). The models that were used in this research are presented below.

2.1 Model 1- Perelson and Nelson (Perelson and Nelson, 1999)

In this first model, in the balance of healthy cells, T, it is assumed that Timo produces healthy cells, T, at a rate, s, and each cell created by Timo reproduces pT healthy cells. In contrast, a death rate is considered of healthy cells equal to $d_T T$, in addition to this rate of death of healthy cells, it is considered that there is a $k_1 VT$ infection rate that reduces the population of healthy cells.

The balance of infected cells, T*, is obtained by balancing cells infected by the action of free viruses at a k1VT rate and infected cells converted to free viruses at a δT* rate.

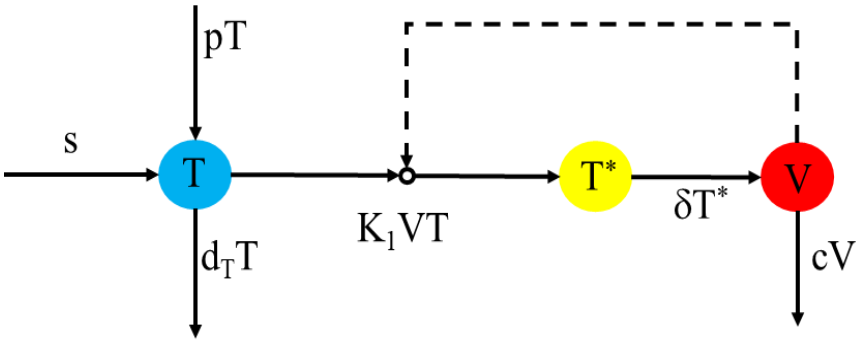
The balance of free virus, V, is performed by accounting for increasing this type of cell at a rate δT* and death at a rate cV. The balance of healthy, infected, and viral cells are presented qualitatively in Figure 1, and the mathematical model for this first model is presented in eqs. (1-3).

$$\frac{dT}{dt} = s - d_T T + pT - k_1 VT \quad (1)$$

$$\frac{dT^*}{dt} = k_1 VT - \delta T^* \quad (2)$$

$$\frac{dV}{dt} = \delta T^* - cV \quad (3)$$

Figure. 1. Balance of cells, healthy, infected, and viral used in model 1.



2.2 Model 2 – Perelson et al. (Perelson, Kirscchner, De Boer, 1993)

The second model to be analyzed has status variables healthy cells, T, infected cells, T*, latently infected cells, T**, and free viruses, V.

In this model, the balance of healthy cells, T, is performed by accounting for healthy cells produced by Timo at a rate s. Each cell produced by Timo reproduces at a rate, pTf (T, T*, T**), which depends on the populations of healthy, infected, latently infected cells and free virus. While similar to model 1, the healthy cell population was considered to have two types of death rates: $d_T T$ and those infected at a $k_1 VT$ rate.

The balance of infected cells, T*, is performed when considering that the $k_1 VT$ rate represents their production. In contrast, two death rates of infected cells, $d_T T^*$ are considered and transformed into latent infected at the $K_2 T^*$ rate.

The balance of latently infected cells is obtained by considering that these cells are produced at the rate $K_2 T$ *, while the death rate of these cells is considered δT**.

V's balance for free viruses differs from model 1, as it considers that each latently infected cell generates N viral cells. Therefore, the rate of production of viral cells is NδT** while the rate of death is represented by cV. The balance of healthy, infected,

latently infected, and viral cells are presented qualitatively in Figure 2, and the mathematical model for this model is presented in eqs. (4-7).

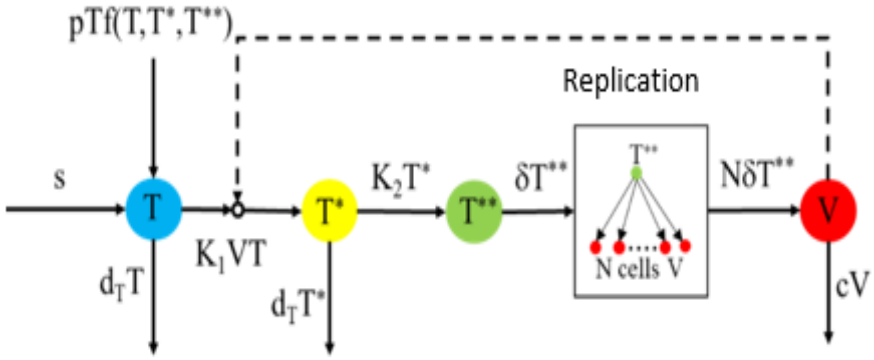
$$\frac{dT}{dt} = s - d_T T + pT\left(1 - \frac{T + T^* + T^{**}}{T_{\max}}\right) - k_1 VT \tag{4}$$

$$\frac{dT^*}{dt} = k_1 VT - d_T T^* - k_2 T^* \tag{5}$$

$$\frac{dT^{**}}{dt} = k_2 T^* - \delta T^{**} \tag{6}$$

$$\frac{dV}{dt} = N\delta T^{**} - k_1 VT - cV \tag{7}$$

Figure. 2. Balance of cells, healthy, infected, latently infected, and viral used in model 2.



2.3 Model 3 – Perelson et al. (Perelson, Kirscchner, De Boer, 1993)

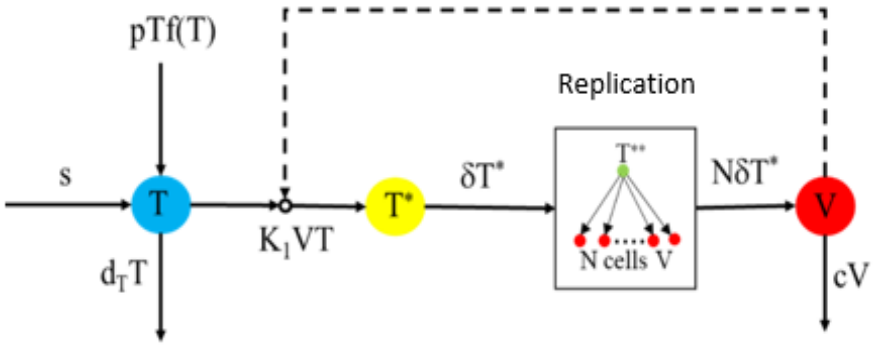
Model 3 is similar to model 1, and the differences are only in the equations to represent the dynamics of healthy and viral cells. While in model 1, there is a production rate pT, in this model, this rate is represented by a logistic function that causes this population to have saturation in T_{max} cells. Regarding viral cells, the difference is that in this model, replication of infected cells is considered. The balance of healthy, infected, latently infected, and viral cells are presented qualitatively in Figure 3, and the mathematical model for this model is presented in eqs. (8-10).

$$\frac{dT}{dt} = s - d_T T + pT\left(1 - \frac{T}{T_{\max}}\right) - k_1 VT \tag{8}$$

$$\frac{dT^*}{dt} = k_1 VT - \delta T^* \tag{9}$$

$$\frac{dV}{dt} = N\delta T^* - cV \qquad (10)$$

Figure. 3. Balance of cells, healthy, infected and viral used in model 3.



The reference parameters and the initial conditions used in the eqs. (1-10) are shown in Tables 1 and 2, respectively.

Table 1. Reference parameters.

Parameters	Value	Unit
s	10	day^{-1} x mm^{-3}
p	0.03	day^{-1}
T_{max}	1500	mm^{-3}
d_T	0.02	day^{-1}
δ	0.24	day^{-1}
c	2.4	day^{-1}
k_1	2.4 x 10^{-5}	mm^3 x day^{-1}
k_2	3.0 x 10^{-3}	day^{-1}
N	1400	Dimensionless

Table 2. Initial conditions.

State variable	Value	Unit
T(0)	10^3	mm^{-3}
T*(0)	0	mm^{-3}
T**(0)	0	mm^{-3}
V(0)	10^{-3}	mm^{-3}

3. APPROXIMATE BAYESIAN COMPUTATIONAL

There are difficulties in obtaining direct measures in several research areas, both for parameters and state variables (Beck and Arnold 1977; Orlande et al., 2011; Kaipio and Somersalo, 2002; Oliveira et al., 2020; Pasqualette et al., 2017). In this scenario, several Bayesian Techniques can be applied to make inferences about the unknown information. In addition to the estimation of parameters, in certain surveys, there are several models to represent a given experimental data, so there is a need also to assess which models make the best inference. There are several Bayesian statistical metrics for comparing models, for example, Akaike, Corrected Akaike, BIC, DIC, TIC (Schwarz, 1978; Konish and Kitagawa, 2008).

Bayesian techniques are based on Bayes' theorem (Schwarz, 1978; Nunes at al., 2021; Moura et al., 2021). However, in such a theorem, it is necessary to model the likelihood equation. However, in several studies, it is not possible to perform repeatability and, therefore, it is impossible to define the likelihood equation (Beaumont, Zhang and Balding, 2002; Marjoram et al., 2003; Beaumont et al., 2009).

The Bayesian Computational Approximation technique does not require the modeling of the likelihood function. It uses another statistical metric to determine whether a sample of models and parameters is accepted or rejected in the algorithm's iterative process.

In this work, the algorithm proposed was an extension of the proposed by Toni et al. (Toni et al., 2009) was based. The adaptations made were in how to determine the tolerance of each population based on the previous population, and for the stopping criterion, the Morozov (1966) principle of discrepancy was adopted (Toni et al., 2009; Toni and Stumpf, 2010; Toni and Stumpf, 2009; Beaumont, Zhang and Balding, 2002; Toni, 2010). The algorithm used is presented:

1. Start regarding free tolerance and define the uncertainties of measurement σ_{pop}^{meas} as:

$$\sigma_{pop}^{meas} = \sum_{i=1}^{N_t} \sigma_i$$

where σ_i is the uncertainty in each time;

2. Define the index to population $pop = 0$;

3. Define index to particle $i = 1$;

4. Sort a model m^* from the probability prior distribution $\pi(m)$. If $pop=1$, sort $\boldsymbol{\theta}^{**}$ that is from the model m^* sorted in the step 4 $\pi(\boldsymbol{\theta}|\, m)$. If $pop>1$, sort $\boldsymbol{\theta}^*$ from the previous population $\left\{\boldsymbol{\theta}\left(m^*\right)_{pop-1}\right\}$ regarding weight $w\left(m^*\right)_{pop-1}$ and perturb the particle $\boldsymbol{\theta}^*$ to obtain $\boldsymbol{\theta}^{**} \sim K_{pop}\left(\boldsymbol{\theta}\,|\,\boldsymbol{\theta}^*\right)$;

5. If $\pi\left(\boldsymbol{\theta}^{**}\right)=0$, go back for step 4;

6. Simulate a candidate data $\mathbf{Y}^* \sim \pi\left(\mathbf{Y}|\boldsymbol{\theta}^{**},\, m^*\right)$. Calculate the tolerance based on the samples of distance accepted in the previous population, $\varepsilon_{pop}=\overline{D}_{pop-1}$. If $d\left(\mathbf{Y}^{exp},\mathbf{Y}^*\right)\geq\varepsilon_{pop}$, go back to step 4;

7. Define $m_{pop}^{(i)}=m^*$ and generate $\boldsymbol{\theta}^{**}$ from the actual population $\left\{\boldsymbol{\theta}\left(m^*\right)_{pop}\right\}$ and calculate the weight of particle $\boldsymbol{\theta}^{**}$,

$$w_{pop}^{(i)}=\begin{cases}1 & if\ pop=1,\\ \dfrac{\pi\left(\boldsymbol{\theta}^{**}\right)}{\sum_{J=1}^{N} w_{pop-1}^{j} K_{pop}\left(\boldsymbol{\theta}_{pop-1}^{(i)},\boldsymbol{\theta}_{pop}^{(i)}\right)}, & \text{if } pop>1\end{cases};$$

8. If $i<N$, define $i=i+1$ and go back to step 4;

9. For each model m, normalize the weight of accepted particle;

10. If $pop<T$, define $pop=pop+1$ and go back for step 3;

11. Define σ_{pop}^{mod} as the uncertainties from the estimations of the model:

$$\sigma_{pop}^{mod}=\sum_{i=1}^{N_t}\sigma_i^{\text{mod}};$$

12. If $\sigma_{pop}^{mod}>\sigma_{pop}^{med}$ go back for step 3. Otherwise, stop.

4. RESULTS AND DISCUSSION

The results will be discussed in two stages. Initially, the reduced sensitivity coefficients for the three models were analyzed, and then the parameter estimates obtained with the different strategies to define the tolerance are discussed. In all cases

analyzed, uncertainty levels of 5% max ($\mathbf{Y}^{\text{Exact}}$) were considered, a priori probability distribution of the parameters being uniform ($U \sim [0 \quad 2\boldsymbol{\theta}^{exact}]$) and 500 particles.

4.1 Reduced sensitivity coefficient

The sensitivity coefficients analysis is essential to obtain precision and accuracy in the estimates (Ozisik and Orlande, 2000). In this analysis, the parameters to be estimated must have a considerable magnitude concerning the state variables measured and linearly independent. Figures 4-6 show the reduced sensitivity coefficients for the three models analyzed.

Figure. 4. Sensitivity coefficient of model 1 in relation to the state variables: (a) T, (b) T*, and (c) V.

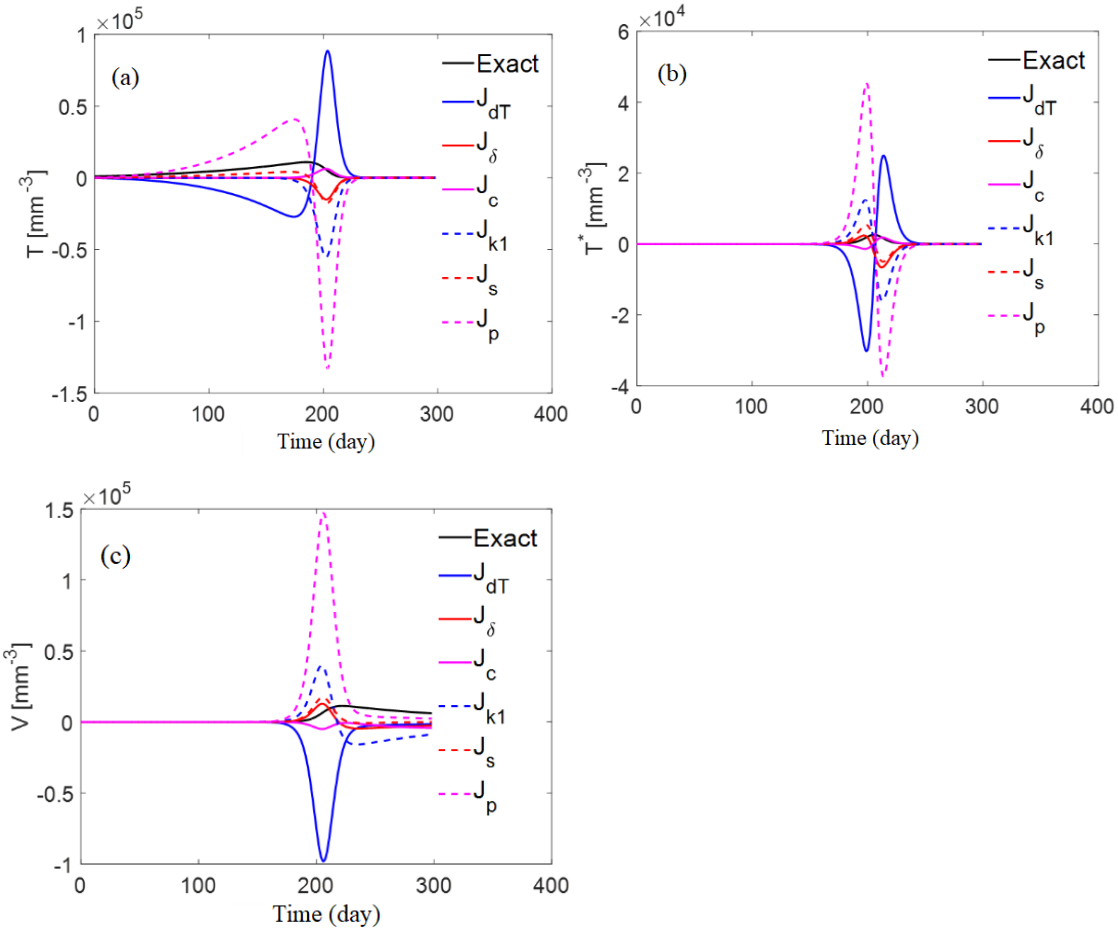


Figure. 5. Sensitivity coefficient of model 2 in relation to the state variables: (a) T, (b) T*, and (c) V.

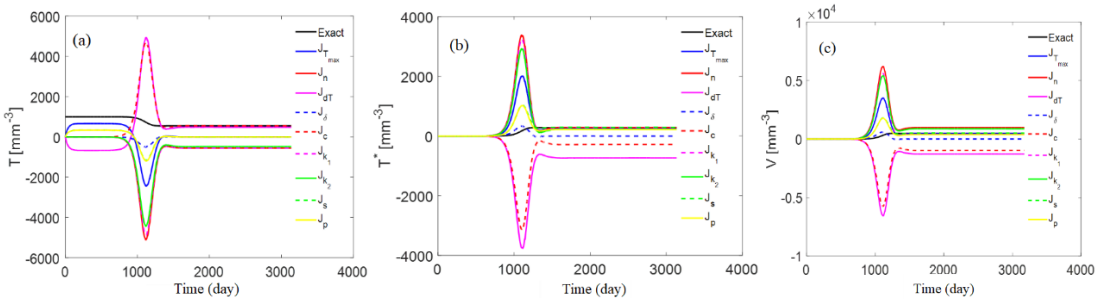
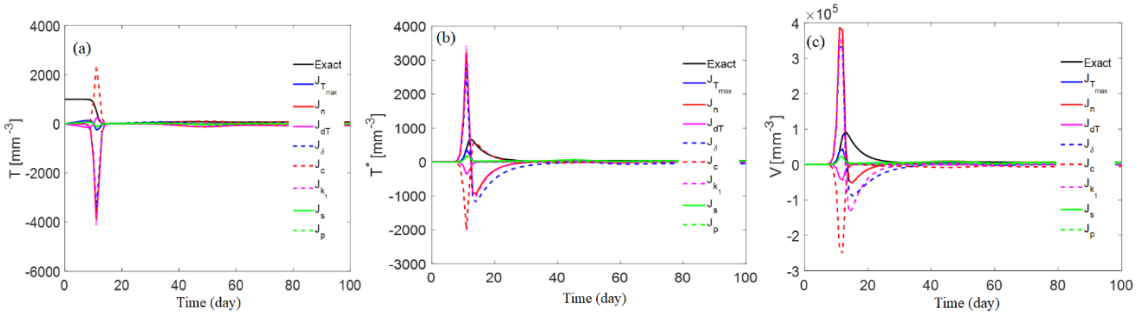


Figure. 6. Sensitivity coefficient of model 3 in relation to the state variables: (a) T, (b) T*, and (c) V.



Figures 4-6 that there are reduced sensitivity coefficients that do not present considerable magnitude for the three models, as well as there is linear dependence. Table 3 summarizes these analyses. There are no markers; it indicates that such reduced sensitivity coefficient does not present considerable magnitude in relation to the measured state variable. The same symbols mean that the reduced sensitivity coefficients are linearly dependent.

Table 3. Analysis of reduced sensitivity coefficients considerable magnitude in relation to the measured state variable. The same symbols mean that the reduced sensitivity coefficients are linearly dependent.

θ	Model 1			Model 2			Model 3		
	T	T*	V	T	T*	V	T	T*	V
T_{max}				XX	XX	XX	XXX	XXX	XXX
N				XX	XX	XX	XXX	OOO	OOO
s	O	O	O	XX	XX	XX	XXX	XXX	XXX
p	X	X	X	XX	XX	XX	XXX	XXX	XXX
d_T	X	X	X	XX	XX	XX	XXX	XXX	XXX
δ	O	O	O	OO	OO	OO	OOO	OOO	XXX
c	O	O	O	XX	XX	XX	OOO	OOO	XXX
k_1	+	X	O	XX	XX	XX	OOO	OOO	XXX
k_2				XX	XX	XX		XXX	XXX

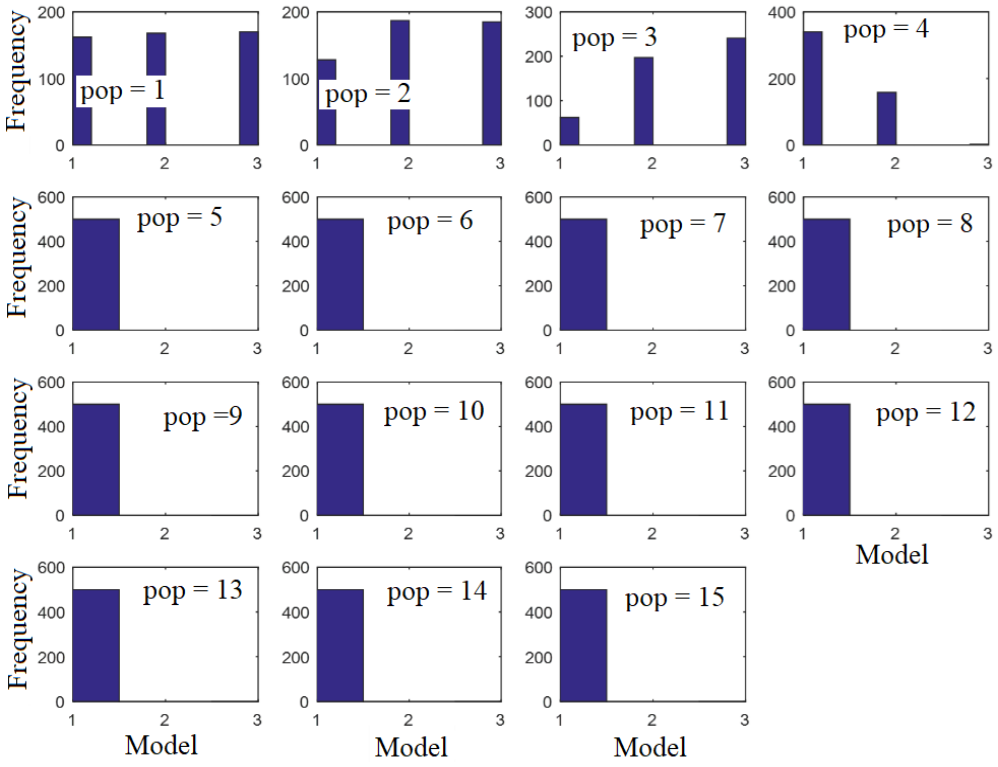
When analyzing Table 3, it is concluded that the following parameters should be estimated for the three models analyzed: $\mathbf{P}_{\mathbf{M1}}^{\mathbf{T}} = [s \;\; p \;\; k_1]$, $\mathbf{P}_{\mathbf{M2}}^{\mathbf{T}} = [N \;\; \delta]$ and $\mathbf{P}_{\mathbf{M3}}^{\mathbf{T}} = [T_{\max} \;\; N \;\; \mathrm{k}_1]$.

4.2 Parameter Estimation and Model Selection - ABC

Parameter estimates and model selection were performed using the Computational Bayesian Approximation technique. An important metric of this method is the definition of the values of the tolerances since this metric is the borderline value (when comparing with the Euclidean distance between the experimental and simulated data) to accept a specific sample of models and parameters. In this work, the tolerance at population (pop) is calculated regarding the mean of the distance related to particles accepted in the previous population.

Initially, the results obtained generating a simulated measure with model 1 and using strategy 1 will be presented since generating a measure with the other models is similar. The selection of models with the evolution of populations is shown in Figure 7.

Figure. 7. Model selection when generating measurements with model 1 and using strategy 1.



When analyzing Figure 7, it appears that in the first population, the three models are equiprobable. It is because it was used as an a priori equiprobable probability distribution for the models.

The three models have a non-zero probability until the third population. In the fourth population, model 3 already has zero probability. Only models 1 and 2 remain in the dispute to better represent the data. However, in the fifth population, the algorithm already determines that the best model to represent the measurements is model 1. However, although the algorithm has already selected the best model, 15 populations were needed for each the adopted stop criterion. It was still necessary to reduce the uncertainties associated with the parameters. Figures 8-10 show the reduction of uncertainties associated with the parameters k_1, s, and p with the populations' advance; one can verify estimates with precision and accuracy compared with the reference parameters (Table 1).

Figure. 8. Estimation of k_1 of model 1.

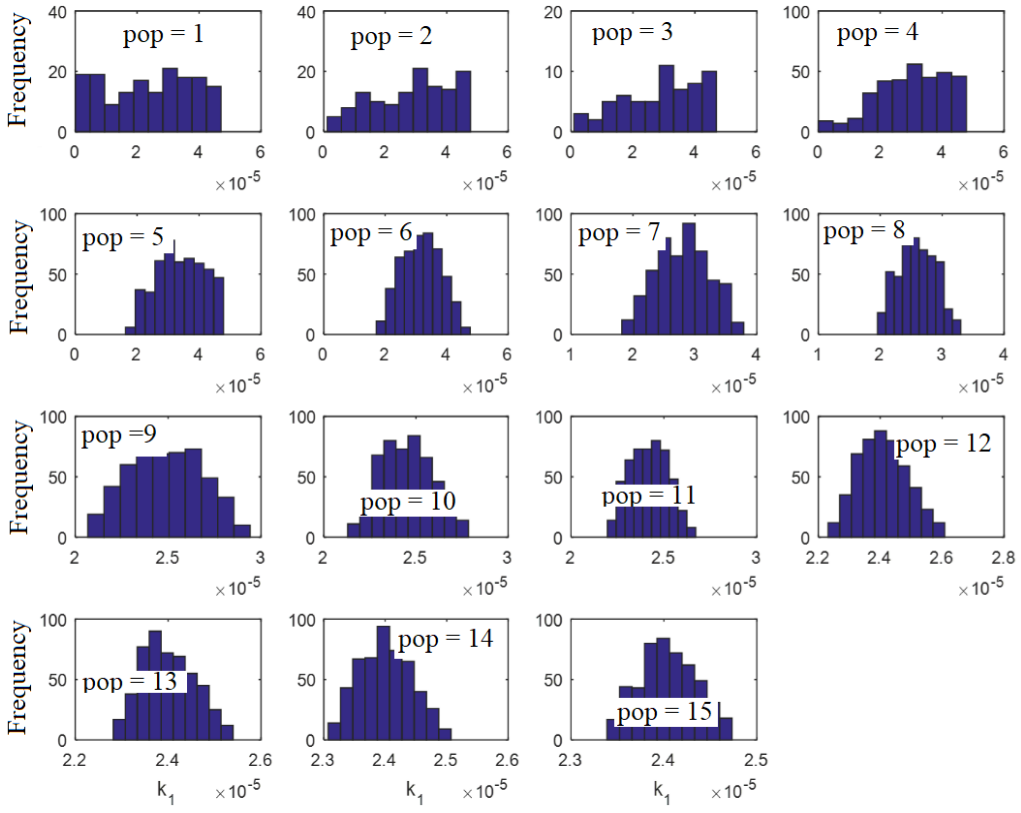


Figure. 9. Estimation of s of model 1.

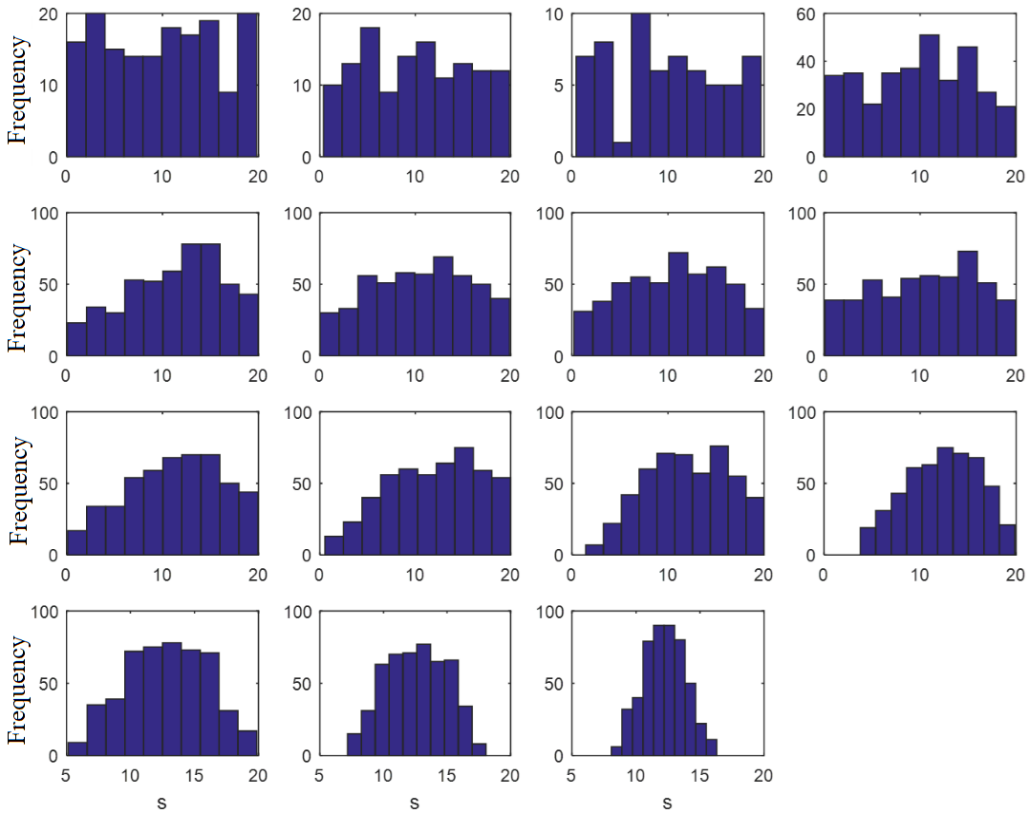
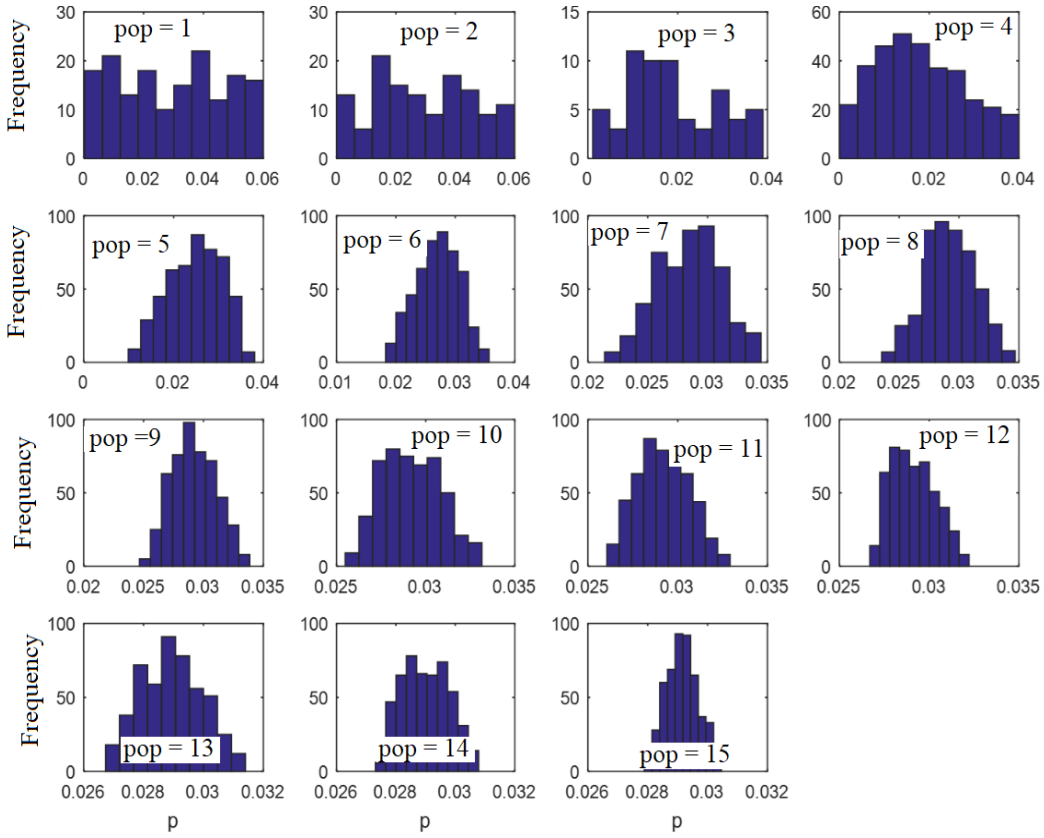


Figure. 10. Estimation of p of model 1.



After analyzing the model selection and parameter estimates, Figures 11-13 show the comparisons of the measured, estimated, and exact state variables (T, T*, and V). It can be seen in Figures 11-12 that in all state variables, in the first population, the estimates do not satisfactorily represent the measures. However, with the advancement of populations, the parameters' uncertainty is reduced and, consequently, the estimates of the state variables are improved.

Figure. 11. Comparisons of the measured, estimated, and exact state variables (T).

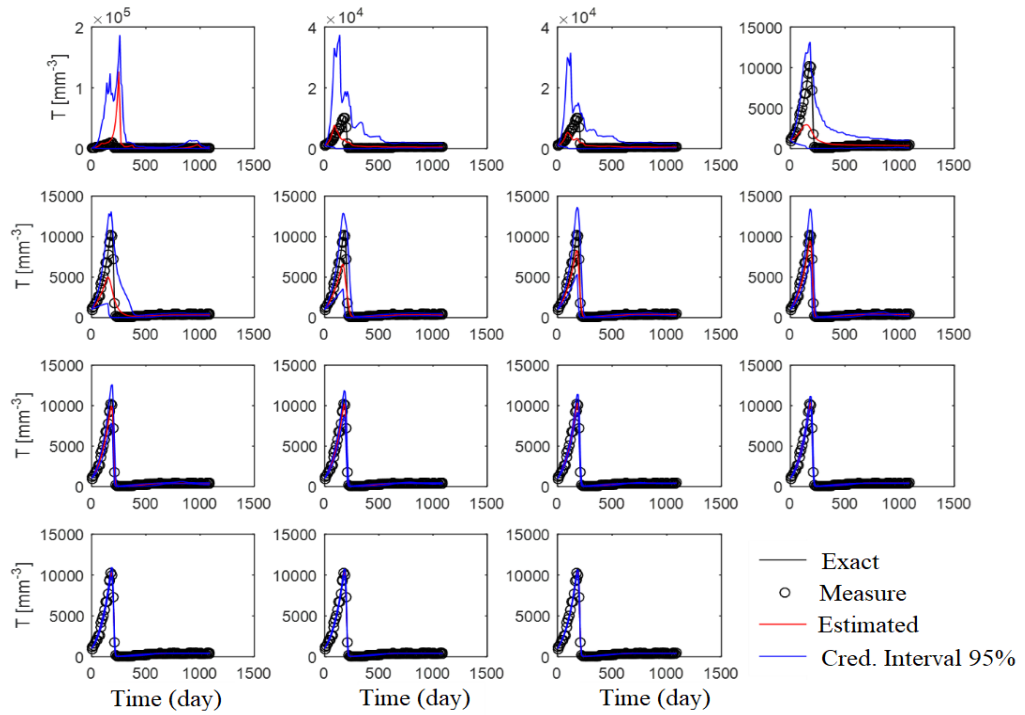


Figure. 12. Comparisons of the measured, estimated, and exact state variables (T*).

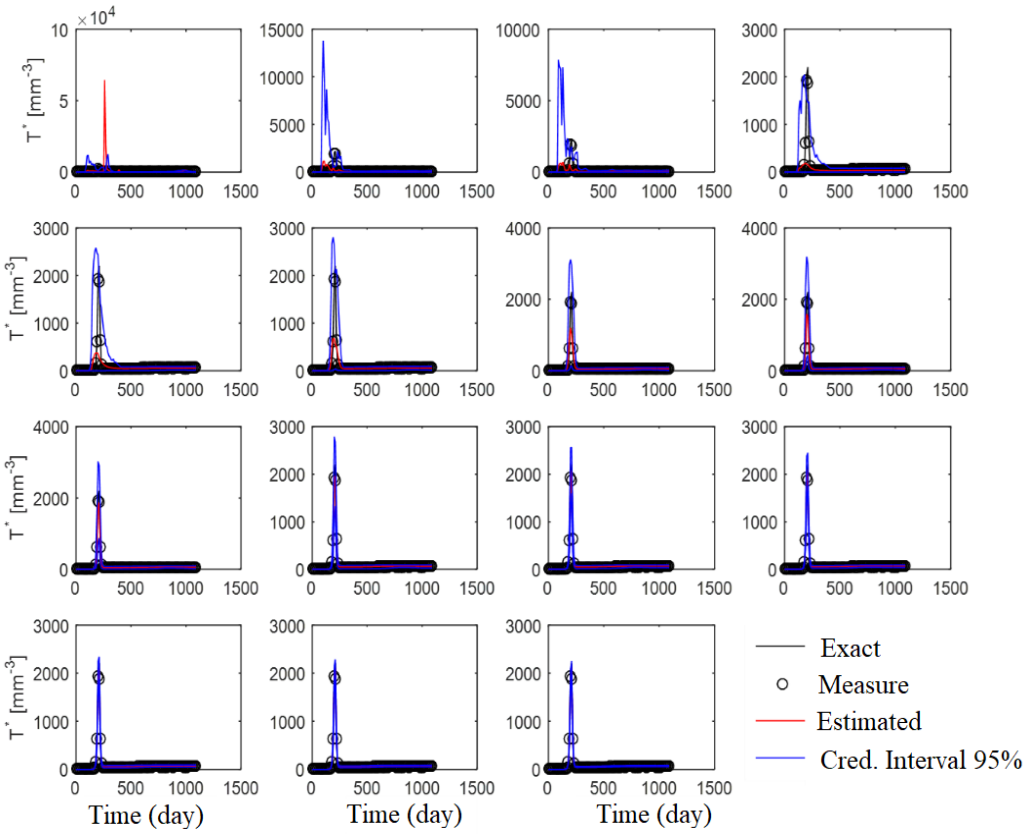
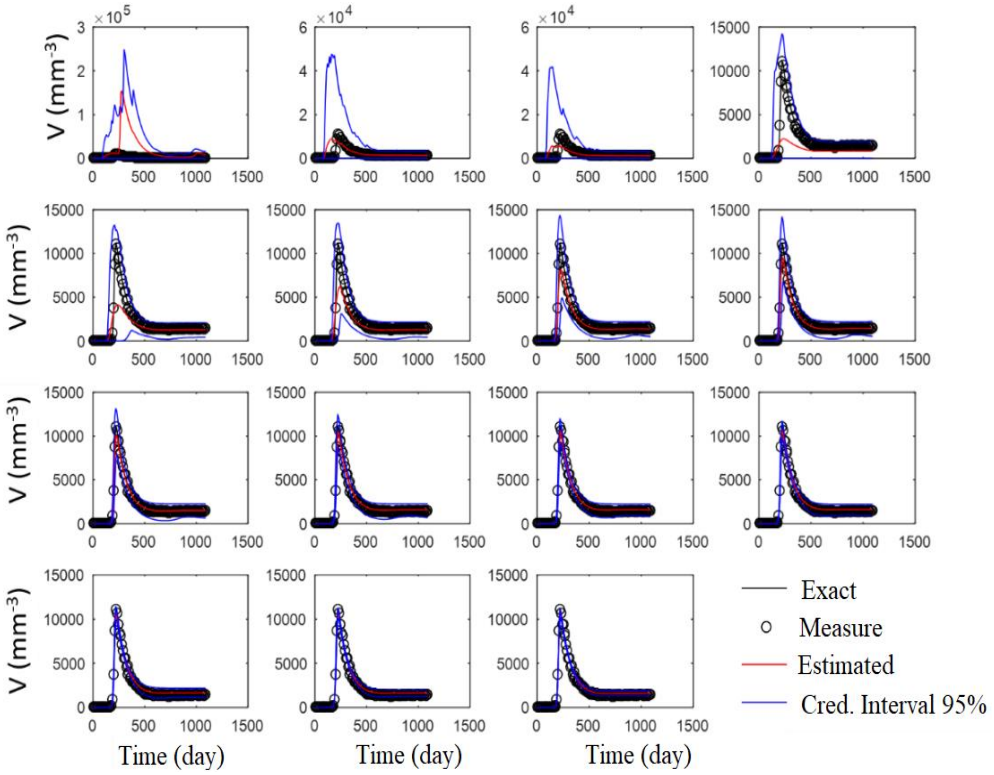


Figure. 13. Comparisons of the measured, estimated, and exact state variables (V).



5. CONCLUSIONS

The use of the Bayesian computational technique proved to be an up-and-coming technique for estimating parameters and selecting models simultaneously.

Initially, a study was carried out in relation to the analysis of the reduced sensitivity coefficients showed that for the three models analyzed it would be possible to estimate the following parameters simultaneously: $\mathbf{p}_{\mathbf{M1}}^{\mathbf{T}} = [s \;\; p \;\; k_1]$, $\mathbf{p}_{\mathbf{M2}}^{\mathbf{T}} = [N \;\; \delta]$ and $\mathbf{p}_{\mathbf{M3}}^{\mathbf{T}} = [T_{\max} \;\; N \;\; k_1]$.

The estimates of the parameters of model 1 were obtained with precision and accuracy. Using simulated measures, it was possible to compare with the reference parameters and prove the algorithm's robustness. In addition to the parameter estimates, excellent T, T *, and V estimates were obtained.

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