Acta Scientiarum

http://periodicos.uem.br/ojs
ISSN on-line: 1807-8664
Doi: 10.4025/actascitechnol.v45i1.56360

STATISTICS

Stanford & Smith nonlinear model in the description of CO_2 evolved from soil treated with swine manure: maximum entropy prior

Edilson Marcelino Silva[1*], Sérgio Alberto Jane[2], Felipe Augusto Fernandes[1], Édipo Menezes da Silva[1], Joel Augusto Muniz[1] and Tales Jesus Fernandes[1]

[1]Programa de Pós-Graduação em Estatística e Experimentação Agropecuária, Departamento de Estatística, Universidade Federal de Lavras, Cx. Postal 3037, 37200-000, Lavras, Minas Gerais, Brazil. [2]Universidade Lúrio, Polo de Niassa, Campus Universitário de Wannangu, Faculdade de Ciências Agrárias, Unango, Sanga, Moçambique. *Author for correspondence. E-mail: edilsonmg3@hotmail.com

ABSTRACT. The dynamics of organic waste decomposition in the soil can be described by nonlinear regression models, however, the theory for regression models is valid for sufficiently large samples, and in general, in small samples, these properties are unknown. One of the methods for data analysis that has been widely used to overcome this problem is the bayesian inference, as it has the advantage of being able to work with small samples, in addition to allowing the incorporation of information from previous studies, and even having a probability distribution for the parameters, consequently, to present a direct interpretation for the credibility interval. However, criticism has been made because of the effect that a prior subjective distribution can have on posterior distribution. One way of determining objective prior is through of maximum entropy prior distributions. For data of organic waste decomposition in the soil, little is known about the probability distributions of the parameters. The present study aimed to use of maximum entropy prior distributions to the parameters of the Stanford & Smith nonlinear model. In addition, using simulated data, to understand the effect that hyperparameters of prior distribution has on the posterior curve, and also to apply the methodology in the description of CO_2 mineralization data from swine manure applied to the soil surface. Data analyzed came from an experiment conducted in a laboratory that evaluated the carbon mineralization of swine manure on the soil surface over time. The posterior distributions were obtained, so the bayesian methodology with maximum entropy prior was efficient in the study of the Stanford & Smith nonlinear model to the data of carbon mineralization of swine manure on the soil surface.

Keywords: bayesian inference; objective prior; decomposition.

Received on October 22, 2020.
Accepted on June 15, 2022.

Introduction

Brazil is the 4th largest pig producer in the world and pig farming is an important agricultural activity with a significant contribution to the national economy (ABPA, 2022). With the increase in pork production, consequently, there is the generation and concentration of a large volume of waste, which requires to reduce the impact of its disposal on the environment. An interesting alternative from the environmental point of view is the disposal of these wastes in agricultural soil as organic matter and source of nutrients for plants (Bison Pinto, Fabbris, Basso, Santi & Girotto, 2014), in addition, protecting the soil from erosion (Doneda et al., 2012). Thus, it is essential to know the process of decomposition and release of nutrients from organic waste in the soil.

The dynamics of waste decomposition plays an important role in the physical, chemical and biological characteristics of the soil. At the beginning of the decomposition of organic waste, easily degradable substances are present, thus, the mineralization of carbon dioxide (CO_2) is greater. Over time, the release of CO_2 decreases, due to mineralization of carbon present in more resistant substances (Pulrolnik, 2009). This process has been described by the nonlinear model of Stanford & Smith (1972), with several residues in the soil (Fernandes et al., 2011; Paula, Silva, Furtado, Fruhauf, & Muniz, 2019; Silva, Ribeiro, Fernandes, & Muniz, 2019a; Silva, Silveira, Ribeiro, & Muniz, 2019b; Nunes, Rodrigues, Barreto, Rodrigues, & Monroe, 2016; Zhou et al., 2012). In addition to presenting a good fit, the Stanford & Smith model is a solution of a differential equation (Sleutel, Neve, Roibás, & Hofman, 2005), thus summarizing the information contained in the data into a few parameters providing values of estimates with useful biological and practical interpretations for producers (Sousa et al., 2014). The Stanford & Smith model, also called first-order kinetic model, is also used to describe nitrogen mineralization (Pereira, Muniz, & Silva, 2005; Pereira, Muniz, Sáfadi, & Silva, 2009; Oliveira, Silva, Muniz, & Savian, 2013; Fernandez, Stolpe, Celis, & Sandoval, 2017; Zhang et al., 2017) and zinc concentration in the soil (Souza, Muniz, Marchi, & Guilherme, 2010; Silva, Furtado, Fruhauf, Muniz, & Fernandes, 2020).

Paula et al. (2020) adjusted the Stanford & Smith model to describe the mineralization of swine manure on the soil surface using the frequentist methodology. A sandy red dystrophic argisol from the 0-10 cm layer was used. Pig slurry showed 31.7 g kg^{-1} dry matter, 9.2 g kg^{-1} carbon and pH of 8.2. Mineralized carbon was evaluated up to 95 days after the start of incubation.

The theory for regression models is asymptotically consistent, that is, it is expected that the larger the sample size, the closer the estimates to the true values of the parameters (Draper & Smith, 1998; Silva et al., 2011; Fernandes, Muniz, Pereira, Muniz, & Muianga, 2015; Carvalho, Beijo, & Muniz, 2017; Sari et al., 2018). However, because of technical limitations, in general, studies deal with few observations, these properties are unknown. One of the methods for data analysis that has been widely used to overcome this problem is the bayesian inference, as it has the advantage of being able to work with small samples, in addition to allowing the incorporation of information from previous studies, and even having a probability distribution for the parameters, consequently, to present a direct interpretation for the credibility interval (Gelman et al., 2014; Machado, Muniz, Sáfadi, & Savian, 2012). The bayesian methodology is based on the Bayes Theorem, whose development is based on conditional probability. According to Bolstad and Curran (2016), the Bayes Theorem can be written in the form of proportionality as:

$$P(B_j|y) \propto P(B_j)L(y|B_j) \quad (1)$$

where $P(B_j)$ is the prior probability for parameters B_j , j = 1, 2, ..., p (where p is the number of model parameters), $L(y|B_j)$ is the likelihood and $P(B_j|y)$ is the posterior probability of parameter B_j.

On the other hand, when little information about prior distribution is available, criticism has been made to the bayesian method because of the effect that prior distribution, possibly subjective, has on inferences, thus, efforts have been made to obtain objective prior distributions (Sorensen & Gianola, 2002). There are several methods of choosing the a priori distribution, such as examples, conjugate prior, Jeffreys prior, among others and according to Jaynes (2003), a way of determining objective prior is through the maximum entropy method, so that people with the same information assign the same prior distribution to the parameter.

For data of organic waste decomposition in soil, scholars have adjusted nonlinear regression models using the frequentist approach, so little is known about the probability distributions of the parameters. Thus, the present study aimed to use of maximum entropy prior distributions in the parameters of the nonlinear Stanford & Smith model. In addition, using simulated data, to understand the effect that prior distribution has on the posterior curve, and also to apply the methodology in the description of CO_2 mineralization data from swine manure applied to the soil surface.

Material and methods

The analyzed data were extracted from Giacomini, Aita, Miola, and Recous (2008) and correspond to the results expressed in means of an experiment that evaluated the carbon mineralization of swine manure on the soil surface, in a completely randomized design with four replications.

The experiment was conducted in a laboratory. A sandy dystrophic argisol was used, from the 0-10 cm layer, of an area that had been managed under no-till system. The soil presented 18 g kg^{-1} organic matter, 150 g kg^{-1} clay and pH in water of 5.2. After sampling, the soil was sieved through a 4 mm mesh and stored in plastic bags for thirteen days before incubation, at room temperature.

Swine liquid manure was obtained from an anaerobic dung from a unit with nursery and breeding animals. The liquid waste contained 46 g kg^{-1} dry matter, 9.7 g kg^{-1} carbon and pH of 7.9. Treatment samples were incubated in acrylic containers. Through the CO_2 emission, carbon mineralization was evaluated, measuring the mineralized carbon at 3, 5, 9, 14, 20, 25, 30, 35, 45, 55, 65, and 80 days from the beginning of the incubation.

To describe carbon mineralization, the Stanford & Smith (1972) model was used with parameterization proposed by Zeviani, Silva, Oliveira, and Muniz (2012):

$$y_i = C_0\left[1 - exp\left(\frac{-ln(2)t_i}{v}\right)\right] + \varepsilon_i$$

where, y_i is the mineralized carbon until time t_i; t_i is the incubation time (in days), with i = 1,2,...,n (where $n = 12$ is the number of days that mineralized carbon was measured); C_0 is the upper horizontal asymptote, that is, potentially mineralizable carbon; v is the time required to mineralize half of C_0, that is, half-life; ε_i is the random error with normal distribution with zero mean and precision $\tau = \frac{1}{\sigma^2}$; ln is the natural logarithm.

Thus, the likelihood for the Stanford & Smith model is written as follows:

$$L(y_i|C_0, v, \tau) \propto \tau^{\frac{n}{2}} exp\left\{\frac{-\tau}{2}\sum_{i=1}^{n}\left\{y_i - C_0\left[1 - exp\left(\frac{-ln(2)t_i}{v}\right)\right]\right\}^2\right\}$$

and can be written matrix-wise as:

$$L(y|C_0, v, \tau) \propto \tau^{\frac{n}{2}} exp\left\{\frac{-\tau}{2}\left(y - C_0\left[1 - exp\left(\frac{-ln(2)}{v}t\right)\right]\right)'\left(y - C_0\left[1 - exp\left(\frac{-ln(2)}{v}t\right)\right]\right)\right\} \quad (2)$$

where

$y = (y_1, y_2, \dots, y_n)'$ and $t = (t_1, t_2, \dots, t_n)'$

Shannon (1948) proposed a quantitative measure of the uncertainty of a probability distribution called information theory entropy or simply called information entropy. For the discrete case, the entropy of information, $H(X)$, of a random variable X is expressed by

$$H(X) = -\sum_{k=1}^{K} p_k log(p_k),$$

where K is the total number of discrete levels. The entropy of information or uncertainty associated with a continuous random variable X tends to infinity, that is, $H(X) \to +\infty$. Thus, for a continuous random variable, the differential entropy, $h(X)$, is defined in analogy to the entropy of information for discrete variables, expressed by

$$h(X) = -\int_{-\infty}^{+\infty} f_X(x) log[f_X(x)]dx$$

where $f_X(x)$ is the probability density function (Haykin, 2007).

The prior distribution should take into account the available information about the parameter and through the maximum entropy method, it is possible to determine the probability distribution with the greatest uncertainty subjected to restrictions that represent the available information (Jaynes, 2003). The maximum entropy method considers the maximization of the differential entropy subjected to the restrictions of a probability density function and its moments, initially known in the distributions and its application involves a restricted optimization problem, and the Lagrange multipliers are used for its solution (Haykin, 2007). Some distributions of maximum entropy with their respective restrictions are listed in Table 1, other distributions and restrictions can be seen in Singh, Rajagopal, and Singh (1986).

Table 1. Some probability distributions and restrictions necessary for their derivation (Koch, 2007).

Distribution	Probability density function	Constraints required
Uniform	$f(x) = \frac{1}{b-a}$	$\int_a^b f(x)dx = 1$
Exponential	$f(x) = \frac{1}{\delta} exp\left(\frac{-x}{\delta}\right)$	$\int_0^{+\infty} f(x)dx = 1$ $\int_0^{+\infty} xf(x)dx = E[x] = \delta$
Truncated normal $(\mathbf{0} \le \boldsymbol{x} \le +\infty)$	$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right)$	$\int_0^{+\infty} f(x)dx = 1$ $\int_0^{+\infty} xf(x)dx = E[x] = \mu$ $\int_0^{+\infty} x^2 f(x)dx = \sigma^2 + \mu^2$

The parameters C_0 and v represent the potentially mineralizable carbon and the half-life time, respectively, and it is expected to have a mean value, moreover, as it moves away from this mean value, the probability decreases, thus it was considered that these parameters have finite variance and can only assume positive values and by Table 1, the prior distribution of maximum entropy for these parameters was the truncated normal:

$$P(C_0|\mu_C,\sigma_C^2) \propto exp\left\{\frac{-1}{2\sigma_C^2}(C_0-\mu_C)^2\right\}, 0 \le C_0 < \infty \qquad (3)$$

$$P(v|\mu_v,\sigma_v^2) \propto exp\left\{\frac{-1}{2\sigma_v^2}(v-\mu_v)^2\right\}, 0 \le v < \infty \qquad (4)$$

For the values of prior distribution parameters, called hyperparameters, we used the estimates obtained by Paula et al. (2020), $\mu_C = 423$ e $\mu_v = 26$. The hyperparameters $\sigma_C^2 = 9025$ and $\sigma_v^2 = 36$ were established so that the prior distributions were consistent with the values of the confidence intervals obtained by the same authors.

The residual standard deviation (RSD) was estimated by Paula et al. (2020) as $R\hat{S}D = \sqrt{Q\hat{M}E} = 40.7$, as σ^2 can be estimated by σ^2= QME, then $\hat{\sigma^2} = 40.7^2$. Since this parameter can only assume positive values and there is a mean value, Table 1 lists the prior distribution of maximum entropy for precision $\tau = \frac{1}{\sigma^2}$, which was the exponential distribution with hyperparameter $\delta = \frac{1}{40.7^2}$:

$$P(\tau|\delta) \propto exp\left\{\frac{-\tau}{\delta}\right\} \qquad (5)$$

There are the likelihood (2) and prior (3), (4) and (5) and through Bayes theorem (1), the joint posterior distribution of the Stanford & Smith model is written as follows:

$$P(C_0, v, \tau|y, \mu_C, \sigma_C^2, \mu_v, \sigma_v^2, \delta) \propto L(y|C_0, v, \tau)P(C_0|\mu_C, \sigma_C^2)P(v|\mu_v, \sigma_v^2)P(\tau|\delta) \qquad (6)$$

In order to make any inference for any model parameter, it is necessary to obtain its marginal posterior distribution. Thus, the joint posterior distribution must be integrated in relation to all other parameters of the model. However, the integration of the joint posterior distribution may not have an analytical expression (Carvalho et al., 2017) and an alternative way to obtain the marginal posterior distributions is through the Gibbs Sampler and Metropolis-Hastings algorithms (Gelman et al., 2014).

The full conditional posterior distribution were obtained from the joint posterior distribution for the implementation of the Gibbs Sampler and Metropolis-Hastings algorithms. With the full conditional posterior, samples of the marginal posterior distributions (chain) were generated using the Gibbs Sampler and Metropolis-Hasting algorithms implemented in the R software (R Core Team, 2020). The convergence of the chains was verified by the criteria of Raftery and Lewis (1992) and Geweke (1992), which are available in the boa package (bayesian output analysis) of the R software (R Core Team, 2020). Through the marginal distributions of each parameter of the model, the mean and the highest posterior density (HPD) interval were calculated.

To demonstrate how changes in the hyperparameter values of the prior distribution affect the posterior curve, y_i values were generated such that:

$$y_i = 550\left(1 - exp\left(\frac{-ln(2)t_i}{25}\right)\right) + e_i$$

where

$$C_0 = 550, v = 25, t = 3,5,9,14,20,25,30,35,45,55,65,80$$

and e_i has a normal distribution with zero mean and precision $\tau = \frac{1}{100}$.

For the simulated data, the hyperparameters of the prior distributions were considered $\mu_C = 400$, $\sigma_C^2 = 1000$, $\mu_v = 35$, $\sigma_v^2 = 3$ and $\delta = \frac{1}{40^2}$. Changes were made to the values of the hyperparameters σ_C^2, σ_v^2 and δ. The isolated effect of each hyperparameter was demonstrated graphically, changing the values of only one hyperparameter and keeping the others constant. As the parameters of the Stanford & Smith model have biological interpretation, the objective was to identify how the change in the values of each hyperparameter changes the posterior curve.

Results and discussion

The inference on each parameter of the Stanford & Smith nonlinear model is carried out by means of marginal distributions of each parameter. Obtaining full conditional posterior distribution is essential for implementing the Gibbs Sampler and Metropolis-Hasting algorithms (Silva, Lima, Silva, & Muniz, 2010; Reis, Muniz, Silva, Sáfadi, & Aquino, 2011; Machado et al., 2012; Prado, Muniz, Savian, & Sáfadi, 2013). From the joint posterior distribution (6) of the Stanford & Smith model, the full conditional posterior distributions (7), (8) and (9) were obtained. It is observed by the expressions (7) and (9) that the full conditional posterior distributions of the parameters C_0 and τ went to the normal and gamma distribution, respectively, and that they depend on the hyperparameters of the prior distribution. As the distributions were known, Gibbs sampling algorithm was applied and for the parameter v, the full conditional posterior (8) was not known, so the Metropolis-Hastings algorithm was used, which obtained approximations of the marginal distributions.

$$P(C_0|v,\tau,y,\mu_C,\sigma_C^2) \propto$$

$$N\left(\frac{\tau y'\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]+\frac{\mu_C}{\sigma_C^2}}{\tau\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]'\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]+\frac{1}{\sigma_C^2}}, \frac{1}{\tau\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]'\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]+\frac{1}{\sigma_C^2}}\right) \quad (7)$$

$$P(v|C_0,\tau,y,\mu_v,\sigma_v^2)\alpha$$

$$\alpha exp\left\{\frac{-\tau}{2}\left(y-C_0\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]\right)'\left(y-C_0\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]\right)-\frac{1}{2\sigma_v^2}(v-\mu_v)'(v-\mu_v)\right\} \quad (8)$$

$$P\left(\tau|C_0,v,y,\frac{1}{\delta}\right)\ G\left(\frac{n}{2}+1,\frac{\left(y-C_0\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]\right)'\left(y-C_0\left[1-exp\left(\frac{-ln\,(2)}{v}t\right)\right]\right)+\frac{2}{\delta}}{2}\right) \quad (9)$$

Figure 1 show how the change in the values of the hyperparameter σ_C^2 affects the posterior curve, keeping the other hyperparameters constant. It can be seen in Figure 1(a - c) that increasing the value of the prior variance σ_C^2, the prior mean $\mu_C = 400$ of the parameter C_0 (upper horizontal asymptote) influences less the posterior mean and tends to the posterior mean of the observed values (in this case, as specified in the material and methods section, the simulated value for the upper horizontal asymptote was 550). Thus, the hyperparameter σ_C^2 determines how the mean μ_C of the prior distribution will influence the estimate of the upper horizontal asymptote. Clearly, if the value of the prior mean μ_C is close to the mean of the observed values, the hyperparameter σ_C^2 will not affect the posterior curve.

Figure 2 illustrates how the change in the values of the hyperparameter σ_v^2 affects the posterior curve, keeping the other hyperparameters constant. It can be seen in Figure 2(a - c) that increasing the value of the prior variance σ_v^2, the prior mean $\mu_v = 35$, of parameter v (half-life time) influences less the posterior mean and tends to the posterior mean of the observed values (in this case, as specified in the material and methods section, the simulated value for the half-life time was 25). Thus, the hyperparameter σ_v^2 defines how the mean μ_v of the prior distribution will influence the half-life time estimate.

Figure 3 demonstrates how the change in the values of the hyperparameter $\delta = \frac{1}{\sigma^2}$ affects the posterior curve, keeping the other hyperparameters constant. When reducing the values of σ^2 (Figure 3(a - c)), the posterior curve tends to approximate the observed values, that is, considering at first that the data show little variability posterior tends to approximate the observed values. Otherwise, posterior tends to an prior curve. In this way, the hyperparameter δ indicates how the observed values will change the posterior curve.

Table 2 lists the results for the analysis of chain convergence of the Stanford & Smith model, adjusted to the data of carbon mineralization of swine manure on the soil surface. The criterion proposed by Geweke (1992) consists of indicating the non-convergence of the posterior mean and presented a p-value greater than 0.05 for all parameters, with no evidence against convergence of the chains. According to the criteria of Raftery and Lewis (1992), the dependence factor (DF) has always presented a value less than five and by the decision rule, it is verified that there is no evidence to reject the non-convergence of the chains. Thus, the use of the Gibbs sampling and Metropolis-Hasting algorithms allowed to obtain integration of posterior densities, making the Bayesian method accessible to researchers from different areas (Firat, Karaman, Basar, & Narinc, 2016).

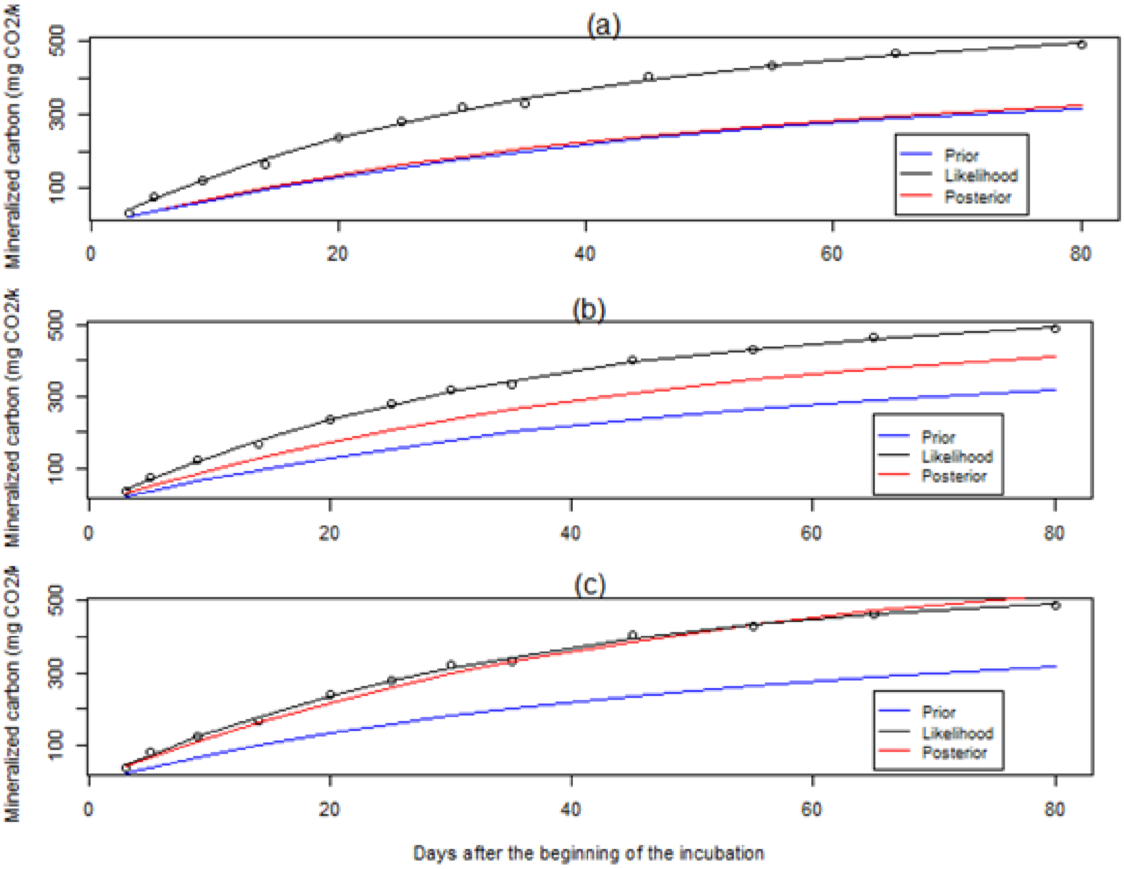

Figure 1. Influence of the parameter σ_C^2 on the posterior curve. Influence of (a) $\sigma_C^2 = 10$, (b) $\sigma_C^2 = 1000$ and (c) $\sigma_C^2 = 10000$, keeping the other parameters constant.

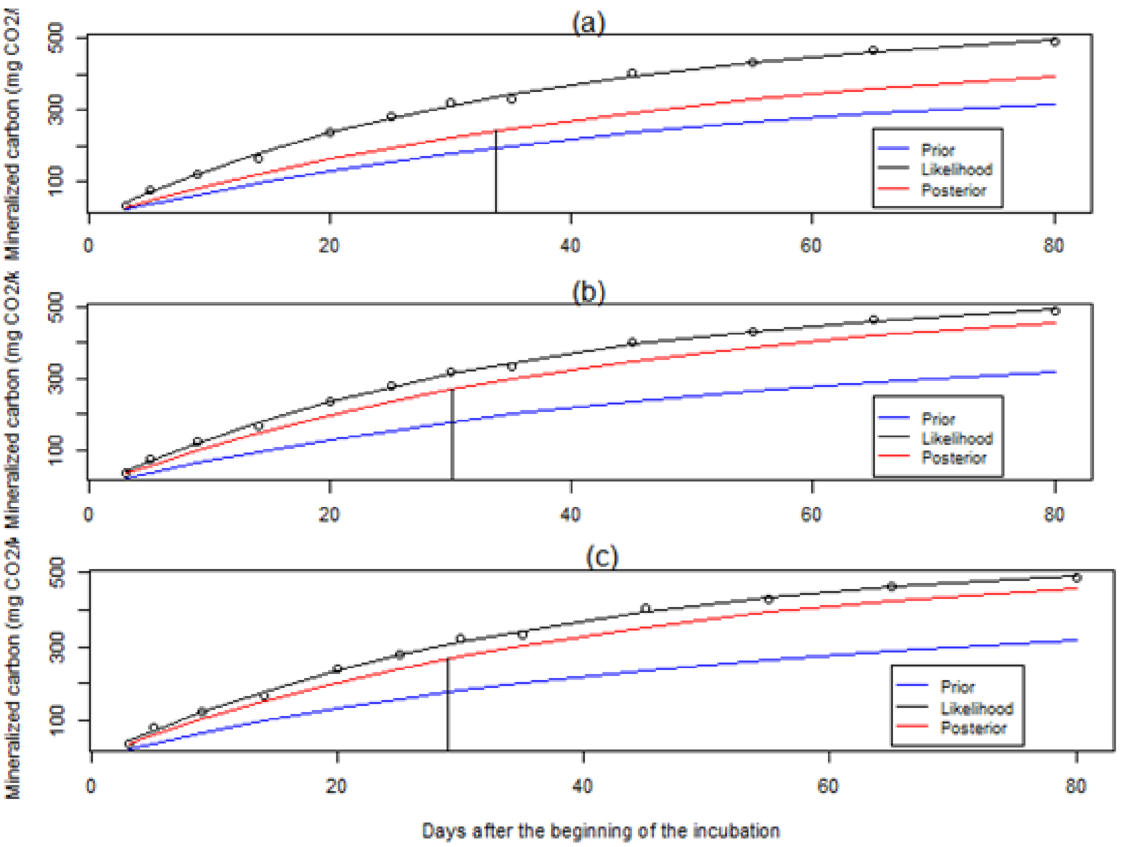

Figure 2. Influence of the parameter σ_v^2 on the posterior curve. Influence of (a) $\sigma_v^2 = 3$, (b) $\sigma_v^2 = 25$ and (c) $\sigma_v^2 = 100$, keeping the other parameters constant. The vertical line indicates the posterior half-life time.

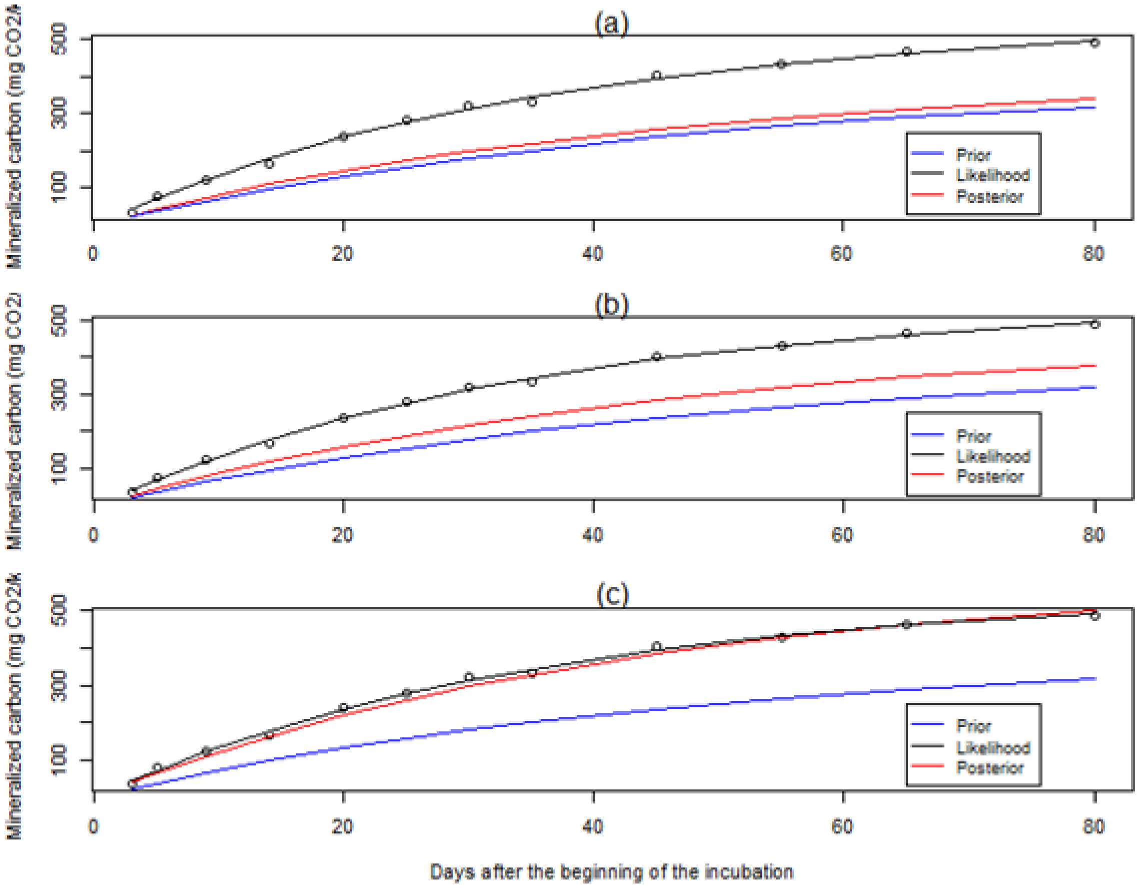

Figure 3. Influence of the parameter δ on the posterior curve. Influence of (a)$\delta = \frac{1}{1000^2}$, (b) $\delta = \frac{1}{100^2}$ and (c) $\delta = \frac{1}{1}$, keeping the other parameters constant.

Table 2. Dependence factor (DF) of the Raftery and Lewis criterion and p-value of the Geweke criterion in the analysis of chain convergence of the Stanford & Smith model, adjusted to the data of carbon mineralization of swine manure on the soil surface.

Parameter	DF	Geweke p-value
C_0	1.0654	0.9183
v	1.4084	0.8202
τ	1.0117	0.1954

Table 3 presents the posterior means with their respective highest posterior density (HPD) for each parameter of the Stanford & Smith model. With the analysis of data of mineralization of swine manure on the soil surface, it was possible to verify that all parameters of the model were significant, since the credibility intervals with 95% probability did not contain zero.

Table 3. A posterior mean of the model parameters and highest posterior density - HPD interval (LL: lower limit and UL: upper limit).

Parameter	Posterior mean	HPD 95%	
		LL	UL
C_0	580.7701	545.7028	613.9485
v	24.9300	22.9640	26.6953
τ	0.0015	0.0004	0.0027

The marginal posterior distributions were obtained (Figure 4), so the Bayesian methodology with maximum entropy prior was an interesting alternative to determine objective prior for the parameters of the Stanford & Smith model, in addition, the Bayesian approach proved to be a viable alternative to overcome the problem of sample size.

The estimates obtained for the parameters of the Stanford & Smith model (Table 3) using the Bayesian approach, were consistent with the estimates obtained by Paula et al. (2020) using the frequentist approach.

The highest posterior density interval (Table 3) with a 95% probability of parameter C_0 was estimated from 545 to 613 mineralized CO_2 mg kg^{-1} and the estimated half-life time (v) from 22 to 26 days. It is important to note that a major advantage of working with the Bayesian methodology is to obtain the highest posterior density (HPD), which is the interval with (1 - α)% probability that contains the most plausible values for the parameter (Guedes, Rossi, Martins, Janeiro, & Carneiro, 2014; Silva et al., 2020).

It can be seen from Figure 4 that the marginal posterior distribution for parameter v was asymmetric to the left, and according to Savian, Muniz, Sáfadi, and Silva (2009) and Silva et al. (2020), in future studies, this information can be considered in an prior distribution. And Figure 5 shows that the observed values had a great influence on the posterior curve.

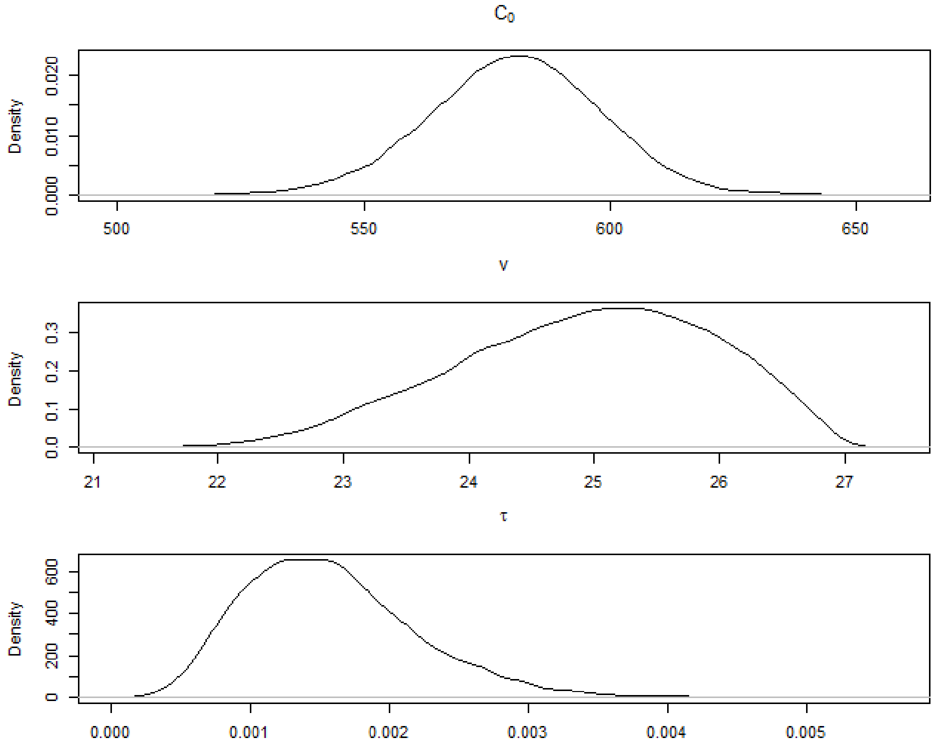

Figure 4. Marginal posterior distributions of each parameter of the Stanford & Smith model.

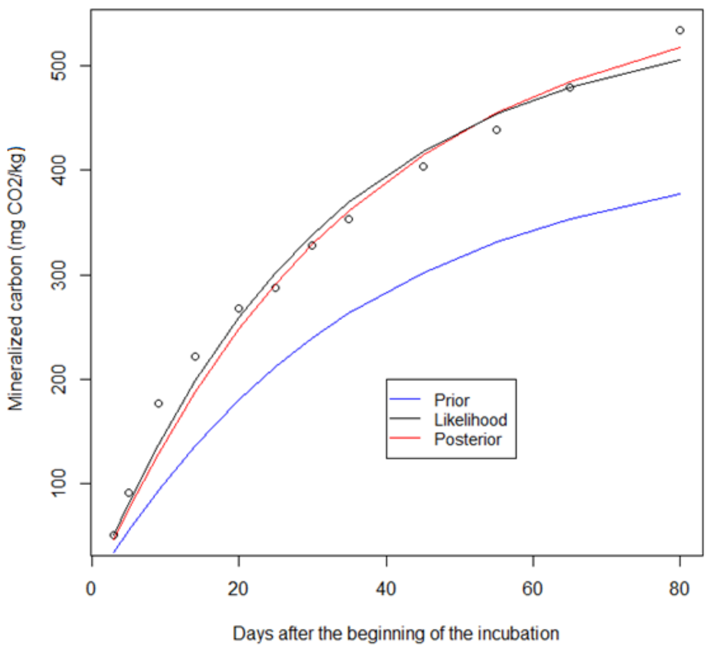

Figure 5. A prior curves, likelihood and a posterior curves of the Stanford & Smith model to the data of swine manure on the soil surface.

Conclusion

The marginal posterior distribution were obtained, indicating that the Bayesian methodology with prior distribution of maximum entropy was an interesting alternative to determine objective prior for the parameters of the Stanford & Smith nonlinear model. Considering the Stanford & Smith model with likelihood (2) and the prior distributions (3), (4) and (5), it was shown that the hyperparameter σ_C^2 defines how the mean $\mu_C$of the prior distribution will influence the estimate of the upper horizontal asymptote, while the hyperparameter σ_v^2 determines how the mean μ_v of the prior distribution will influence the half-life time estimate and the hyperparameter δ describes how the observed values will affect the posterior curve.

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