

Gompertz model describing CO₂ evolved from legumes in the soil: bayesian approach with maximum entropy prior

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ABSTRACT. For residues maintained on the soil surface, microbial colonization of the substrate is slower initially due to the microbial population's adaptation phase to the substrate. Subsequently, decomposition becomes more intense due to easily mineralizable matter, and as the process progresses, there is a predominance of more resistant materials that can reduce microbial attack. Thus, the maximum rate of CO₂ release occurs in the early days of decomposition, and this process is described by the Gompertz model, which is a nonlinear sigmoidal regression model. The theory for regression models is valid for sufficiently large samples, and generally, in research with carbon mineralization data, few observations are used, and parameter estimation should preferably be done using Bayesian methodology since prior information is incorporated, reducing the effect of having few observations. One way to determine objective priors is through maximum entropy prior distributions. This study aims to fit the Gompertz model to the release of carbon dioxide over time from leguminous species using a Bayesian approach with maximum entropy priors for the model parameters. The treatments (leguminous species) evaluated were *Arachis pinto*i, *Calopogonium mucunoides*, *Stylosanthes guianensis*, and *Stizolobium aterrium*. Eight observations of carbon released over time up to 480 hours from the start of incubation were made. In the soil with the addition of legumes, the abscissa of the inflection point was estimated between 4 and 5 days, meaning this was the time the microorganisms needed to reach the maximum decomposition rate. The species *A. pinto*i showed the average estimate of 481 mg CO₂ of potentially mineralizable carbon, being the species that released the most carbon.

Keywords: nonlinear model; bayesian inference; objective prior; decomposition.

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Introduction

The use of soils in agriculture as decreased their productive capacity due to degradation, requiring the inclusion of organic matter to maintain their production potential (Matos et al., 2008; Pereira, Soares, & Miranda, 2016; Silva, Frühauf, Silva, Muniz, Fernandes, 2023a). Using legumes as cover crops has been an interesting alternative, since the inclusion of residues in the soil can control soil moisture and temperature as well as release macronutrients and micronutrients for crops (Rodrigues et al., 2012), understanding the process of nutrient release from organic residues added to the soil over time is important to increase soil productivity in order to meet the crop demand (Silva, Ribeiro, Fernandes, & Muniz, 2019a; Silva, Silveira, Ribeiro, Muniz, 2019b).

According to Matos et al. (2008) and Giacomini, Aita, Miola, and Recous (2008), the decomposition process is slow initially due to the microbial adaptation phase to the soil residue, followed by intense mineralization due to the availability of materials that are easily decomposed, and then a phase more resistant to mineralization due to the quantity and composition of the available residues that can reduce the microbial mineralization process. This decomposition dynamics can be described by the nonlinear regression model Gompertz (Silva et al., 2023a), which is a sigmoidal model (Matos et al., 2008; Monteiro, Cantarutti, Nascimento Junior, Regazzi, & Fonseca, 2002), and since it exhibits an inflection point at the beginning of the curve, it is suitable for describing this process of organic residue mineralization in soil.

The theory for regression models is valid for sufficiently large samples, meaning they are asymptotically consistent (Draper & Smith, 1998; Sari et al., 2018; Carvalho, Beijo, & Muniz, 2017; Silva et al., 2023b). However, due to technical limitations, research generally deals with few observations, and parameter estimation should preferably use the Bayesian methodology. This is because it incorporates prior information,

reducing the impact of a few observations. Furthermore, having probability distributions for the parameters and being able to obtain the credibility interval with the most plausible values for each of the parameters (Bolstad & Curran, 2016; Gelman et al., 2014; Fernandes, Pereira, Bueno Filho, & Muniz, 2022).

However, as the prior distribution is subjective when little information is available regarding the parameter, questions have been raised because this distribution will influence posterior inference. Thus, efforts have been made to obtain objective prior distributions (Sorensen & Gianola, 2002; Haykin, 2007). According to Jaynes (2003), the maximum entropy method is an alternative to reduce this subjectivity. In this method, considering the knowledge of some moments of the distribution as well as its parameter space, individuals with the same information will assign the same prior distribution to the parameter under study, while also maximizing entropy

This study aimed to fit the Gompertz model using the Bayesian approach with maximum entropy priors for the model parameters, we investigated the carbon dioxide mineralization over time for the following leguminous species in soil: *Arachis pintoii*, *Calopogonium mucunoides*, *Stylosanthes guianensis*, and *Stizolobium aterrimum*. Additionally, based on the model, we inferred the potentially mineralizable carbon and the time required for microorganisms to reach maximum decomposition rate.

Material and methods

The experiment was conducted from December 2003 to April 2004 in partnership with UFV/EPAMIG/CTA (data obtained from Matos et al., 2008). The leguminous species were obtained from family farmers in the municipality of Pedra Dourada, located in the Zona da Mata region of the state of Minas Gerais.

The soil used had a clayey texture and was classified as Red-Yellow Latosol. The soil had the following attributes: pH (H₂O) of 5.0; Al³⁺ of 1.0, Ca²⁺ of 0.48, and Mg²⁺ of 0.14 cmol_c dm⁻³; available P and K (Mehlich⁻¹) of 2.4 and 56 mg dm⁻³, respectively; and organic carbon content of 36 g kg⁻¹ (Walkey-Black). For soil correction, 1.20 t ha⁻¹ of limestone, 300 kg ha⁻¹ of gypsum, 125 kg ha⁻¹ of potassium sulfate, and 800 kg ha⁻¹ of thermophosphate were applied.

Four leguminous species (treatments) used in green manure were evaluated: *Arachis pintoii* (amendoim forrageiro), *Calopogonium mucunoides* (calopogônio), *Stylosanthes guianensis* (mineirão) and *Stizolobium aterrimum* (mucuna), cultivated in the inter-rows of coffee plants. Four months after planting (flowering stage), the aboveground parts of the legumes were collected. The treatments, after being dried in an oven, ground, and passed through a 2 mm sieve, were chemically and biochemically characterized. A randomized block design with four blocks was used.

Through respirometry assay, the evolution of CO₂ was measured using a continuous flow respirometer. Eight measurements of evolved CO₂ were taken over the days, with the first five measurements every 48 hours, two every 72 hours, and the last one at 96 hours, totaling 480 hours. The Gompertz model was fitted to the CO₂ evolutions, expressed as a function of time (hours), according to the parameterization indicated by Fernandes, Muniz, Pereira, Muniz, and Muianga (2015):

$$y_i = C_0 e^{-e^{k(\beta - t_i)}} + \varepsilon_i,$$

where e is exp; y_i is the mineralized carbon at time t_i ; t_i is the incubation time (in hours), with $i = 1, 2, \dots, n=8$; the parameter C_0 represents the upper horizontal asymptote and practically indicates the potentially mineralizable carbon, while β indicates the abscissa of the inflection point, that is, the time required for microorganisms to reach the maximum mineralization rate. The parameter k indicates the CO₂ evolution constant (Jane et al., 2020). The magnitude of the parameters C_0 and β reflects the degradability of the legume and microbial activity, respectively. In turn, ε_i is the random error, assumed to have a normal distribution with a mean of 0 and precision $\tau = \frac{1}{\sigma^2}$, meaning $\varepsilon_i \sim N(0, \tau)$ (Pagnoncelli Junior, Trezzi, Salomão, Gonzalez-Andujar, 2021; Abrantes et al., 2019). According to Fernandes et al. (2015), in this parameterization of the Gompertz model, it is possible to show the inflection point occurs at coordinates $(\beta, \frac{C_0}{e})$.

The likelihood for the Gompertz model is written as follows:

$$L(y_i | C_0, \beta, k, \tau) \propto \tau^{\frac{n}{2}} \exp \left\{ -\frac{\tau}{2} \sum_{i=1}^n \left\{ y_i - C_0 e^{-e^{k(\beta - t_i)}} \right\}^2 \right\},$$

where α is proportional and can be written in matrix form as:

$$L(\mathbf{y}|\mathbf{C}_0, \beta, k, \tau) \propto \tau^{\frac{n}{2}} \exp \left\{ \frac{-\tau}{2} \left(\mathbf{y} - \mathbf{C}_0 e^{-e^{k(\beta-t)}} \right)' \left(\mathbf{y} - \mathbf{C}_0 e^{-e^{k(\beta-t)}} \right) \right\}, \quad (1)$$

where $\mathbf{y} = (y_1, y_2, \dots, y_n)'$ and $\mathbf{t} = (t_1, t_2, \dots, t_n)'$.

The parameters \mathbf{C}_0 and β represent the potentially mineralizable carbon and the abscissa of the inflection point, respectively. It was assumed that they have finite mean, variance, and can only take positive values, and the maximum entropy prior distribution for these parameters with these constraints was the truncated normal distribution (Silva et al., 2023a; Singh, Rajagopal, & Singh, 1986):

$$P(\mathbf{C}_0|\mu_C, \sigma_C^2) \propto \exp \left\{ \frac{-1}{2\sigma_C^2} (\mathbf{C}_0 - \mu_C)^2 \right\}, 0 \leq \mathbf{C}_0 < \infty \text{ and } \sigma_C^2 > 0. \quad (2)$$

$$P(\beta|\mu_\beta, \sigma_\beta^2) \propto \exp \left\{ \frac{-1}{2\sigma_\beta^2} (\beta - \mu_\beta)^2 \right\}, 0 \leq \beta < \infty \text{ and } \sigma_\beta^2 > 0. \quad (3)$$

Parameter k represents the CO_2 evolution constant, which is generally expected to fall within the range of 0 to 1 and follows a right-skewed distribution (Silva et al., 2023a; Silva et al., 2022b). In this case, the maximum entropy prior distribution for this parameter was a beta distribution (Singh et al., 1986):

$$P(k|a, b) \propto k^{a-1} (1-k)^{b-1}, 0 < k \leq 1. \quad (4)$$

The residual standard deviation (RSD) is estimated by $RSD = \sqrt{MSE}$, and σ^2 can be estimated by $\sigma^2 = MSE$, where MSE is the mean squared error. Since this parameter has a mean value and can only take positive values, the maximum entropy prior distribution for precision τ was the exponential distribution (Silva et al., 2023a; Singh et al., 1986):

$$P(\tau|\delta) \propto \exp \left\{ \frac{-\tau}{\delta} \right\}, \tau \geq 0 \text{ and } \delta > 0. \quad (5)$$

We have the likelihood (1) and the priors (2), (3), (4), and (5), and through Bayes' theorem (Bolstad & Curran, 2016), the joint posterior distribution is proportional to:

$$P(\mathbf{C}_0, \beta, k, \tau|\mathbf{y}, \mu_C, \sigma_C^2, \mu_\beta, \sigma_\beta^2, a, b, \delta) \propto L(\mathbf{y}|\mathbf{C}_0, \beta, k, \tau) P(\mathbf{C}_0|\mu_C, \sigma_C^2) P(\beta|\mu_\beta, \sigma_\beta^2) P(k|a, b) P(\tau|\delta). \quad (6)$$

Values of hyperparameters for the prior distributions were obtained based on the literature (Silva et al., 2023a; Matos et al., 2008). The estimates were used as means, and the dispersion hyperparameters were obtained on the parameter intervals.

From the joint posterior distribution (6) and with algebraic calculations, the complete conditional posterior distributions were obtained. When the complete conditional posterior was known, the Gibbs Sampler was used to obtain samples from the marginal posterior distribution, and when it was not possible to associate it with the kernel of any known distribution, the Metropolis-Hastings algorithm was used to obtain samples from the marginal posterior distribution. Samples from the marginal posterior distributions (chain) were generated using the Gibbs Sampler and Metropolis-Hastings algorithms implemented in the R software (R Core Team, 2023). The convergence of the chains was checked using the Raftery and Lewis (1992) and Geweke (1992) criteria, which are available in the *boa* (Bayesian Output Analysis) package of the R software (R Core Team, 2023). The mean, mode, and highest posterior density (HPD) interval were calculated.

Results and discussion

Through Bayes theorem, complete conditional posterior distributions were obtained, which are necessary for the implementation of the Gibbs Sampler and Metropolis-Hastings algorithms (Machado, Muniz, Sáfiadi, & Savian, 2012; Prado, Muniz, Savian, & Sáfiadi, 2013; Silva et al., 2022a) to make inferences for each marginal posterior distribution of the parameter of the nonlinear Gompertz regression model. From the joint posterior distribution (6) of the Gompertz model, complete conditional posterior distributions (7), (8), (9), and (10) were obtained. From expressions (7) and (10), it can be observed that the complete conditional posterior distributions of the parameters indicating potentially mineralizable carbon (\mathbf{C}_0) and precision (τ) were normal and gamma distributions, respectively. When the core of the conditional posterior distribution is known, it is possible to implement the Gibbs sampler to obtain samples from the marginal distributions. However, for the

parameters indicating the abscissa of the inflection point (β) and the carbon mineralization rate (k), the complete conditional posterior distributions (8) and (9) were not known. In these cases, the Metropolis-Hastings algorithm was implemented to obtain approximations of the marginal posterior distributions (Gelman et al., 2014).

$$P(C_0 | y, \beta, k, \tau, \mu_C, \sigma_C^2) \sim$$

$$N \left(\frac{\tau y e^{-e^{k(\beta-t)}} + \frac{\mu_C}{\sigma_C^2}}{\frac{\tau}{(e^{-e^{k(\beta-t)}})^{\frac{1}{\sigma_C^2}}} + \frac{1}{\sigma_C^2}}, \frac{1}{\frac{\tau}{(e^{-e^{k(\beta-t)}})^{\frac{1}{\sigma_C^2}}} + \frac{1}{\sigma_C^2}} \right) \quad (7)$$

$$P(\beta | y, \alpha, k, \tau, \mu_\beta, \sigma_\beta^2) \propto \exp \left\{ \frac{-\tau}{2} (y - \alpha e^{-e^{k(\beta-t)}})' (y - \alpha e^{-e^{k(\beta-t)}}) - \frac{1}{2\sigma_\beta^2} (\beta - \mu_\beta)' (\beta - \mu_\beta) \right\} \quad (8)$$

$$P(k | y, \alpha, \beta, \tau, a, b) \propto$$

$$k^{a-1} (1-k)^{b-1} \exp \left\{ \frac{-\tau}{2} (y - \alpha e^{-e^{k(\beta-t)}})' (y - \alpha e^{-e^{k(\beta-t)}}) \right\} \quad (9)$$

$$P(\tau | y, \alpha, \beta, k, \delta) \sim G \left(\frac{n}{2} + 1, \frac{(y - \alpha e^{-e^{k(\beta-t)}})' (y - \alpha e^{-e^{k(\beta-t)}}) + \frac{2}{\delta}}{2} \right) \quad (10)$$

As observed by Silva et al. (2022a) and indicated by expression (7), it can be noted that the hyperparameter of the prior mean μ_C has as its denominator the hyperparameter of the prior variance σ_C^2 , and increasing the value of σ_C^2 will not influence the prior mean to posterior mean of the parameter C_0 , meaning that the posterior of the parameter will be influenced only by the data. For parameter β , hyperparameters σ_β^2 and μ_β mostly similarly influence the posterior.

In Table 1, the p-value of the Geweke criterion (1992) is presented, as well as the dependence factor (FD) of the Raftery and Lewis criterion (1992) for the Gompertz model. Since the p-value of the Geweke criterion is greater than 0.05, there is no evidence against the convergence of the chains. Similarly, the dependence factor (FD) always obtained a value less than 5, and there was no evidence to reject the non-convergence of the chains (Silva et al., 2022a). Therefore, using Gibbs Sampler and Metropolis-Hastings algorithms allowed for obtaining posterior density integration (Gelman et al., 2014), making the Bayesian method accessible (Firat, Karaman, Basar, & Narinc, 2016).

Table 1. Raftery and Lewis criterion (Dependence factor - DF) and Geweke criterion (p-value) in the analysis of chain convergence.

Treatment	Parameter	DF	Geweke p-value
Soil	C_0	1.0072	0.9604
	β	1.0993	0.8368
	k	2.2303	0.2550
	τ	0.9826	0.1847
<i>S. atterrimum</i>	C_0	1.0157	0.4595
	β	1.1895	0.3429
	k	2.0758	0.6491
	τ	0.9786	0.0535
<i>S. mucunoides</i>	C_0	1.0282	0.4276
	β	1.2562	0.8989
	k	1.9001	0.3871
	τ	0.9906	0.2061
<i>S. guianensis</i>	C_0	1.0306	0.7189
	β	1.4263	0.9679
	k	2.1356	0.2884
	τ	1.0032	0.5599
<i>A. pintoii</i>	C_0	1.0157	0.7435
	β	1.0947	0.9246
	k	2.1460	0.8431
	τ	1.0032	0.5713

Source: Prepared by the authors (2024).

Table 2 presents the posterior mean and mode with their respective 95% highest posterior density (HPD) intervals for each parameter of the Gompertz model. The analysis of legume mineralization data in the soil

indicated that all model parameters were significant, because the credibility intervals with 95% probability had the lower limit and the upper limit greater than zero.

Table 2. A posterior mean and posterior mode of the model parameters and highest posterior density (HPD) interval (LL: lower limit and UL: upper limit).

Treatment	Parameter	Mode	LL	Mean	UL
Soil	C_0	15.8575	15.1525	15.8132	16.4218
	β	73.5680	72.9538	73.5954	74.2443
	k	5.39e-04	2.5 e-07	8.576 e-03	4.26338 e-02
	τ	0.0341	0.00509	0.11483	0.40782
<i>S. atterrimum</i>	C_0	408.4185	384.6591	406.4399	427.8216
	β	111.999	111.6029	112.0002	112.3836
	k	5.888 e-04	1.23 e-07	9.193 e-03	4.6386 e-02
	τ	8.455 e-05	4.846 e-06	3.045 e-04	8.692 e-04
<i>S. mucunoides</i>	C_0	419.4693	395.1673	418.6630	442.1772
	β	115.9648	115.6032	115.9973	116.3734
	k	6.16 e-04	6 e-08	9.288 e-03	4.6201 e-02
	τ	7.86 e-06	5.74 e-06	2.89 e-04	8.46 e-04
<i>S. guianensis</i>	C_0	454.2005	430.3974	454.5122	478.2225
	β	115.0231	114.6760	115.0002	115.3237
	k	6.866 e-04	6.1 e-08	9.046 e-03	4.5149 e-02
	τ	6.441 e-05	5.09 e-06	2.493 e-04	6.9696 e-04
<i>A. pintoi</i>	C_0	482.3409	460.0091	481.4390	502.5491
	β	119.0281	118.5148	119.0008	119.5035
	k	4.96 e-04	1.95 e-07	8.772 e-03	4.4954 e-02
	τ	4.656 e-05	2.748 e-06	2.324 e-04	5.933 e-04

Source: Prepared by the authors (2024).

Based on the credibility intervals shown in Table 2, legumes can be grouped according to their potentially mineralizable carbon (parameter C_0). There was no overlap in the credibility intervals of the C_0 parameter between the soil and other treatments. Therefore, adding legumes to the soil increased the carbon mineralization of legumes in the soil (Paula, Silva, Furtado, Frühauf, & Muniz, 2019; Fernandes et al., 2011). The *A. pintoi* treatment had a higher amount of potentially mineralizable carbon than the other treatments. Additionally, there was overlap in the credibility intervals of the C_0 parameter for the treatments *S. atterrimum*, *S. mucunoides*, and *S. guianensis*, indicating that the amount of potentially mineralizable carbon in these treatments did not differ significantly, as also observed by Matos et al. (2008) and Silva et al. (2022a).

The parameter β indicates the abscissa of the inflection point, and in the Gompertz model, it occurs when potentially mineralizable carbon reaches 37% of its capacity (Pagnoncelli Junior et al., 2021; Sari et al., 2018; Fernandes et al., 2015), which practically indicates how many hours are needed to reach the maximum point of mineralization, related to microbial activity. The maximum mineralization rate of the legume treatments occurred between approximately 112 and 119 hours (β estimate - Table 2), i.e., between the 4th and 5th day, and these results are in accordance with those obtained by Silva et al. (2022a). Conversely, Matos et al. (2008) found later estimates, which is due to the authors using the Logistic model, which is not suitable, as it is observed that the maximum mineralization rate occurs at the beginning of the process (Silva et al., 2022a; Giacomini et al., 2008).

The marginal posterior distributions were obtained and are presented in Figures 1, 2, 3, 4, and 5. Bayesian inference with maximum entropy prior was an appropriate methodology to overcome the problem of sample size. The marginal posterior distribution for parameters C_0 and β is symmetric, while for parameters k and τ , they were right-skewed distributions. According to Savian, Muniz, Sáfiadi, and Silva (2009) and Silva et al. (2020), in future studies, this information can be considered in the prior distribution of these parameters.

The posterior mean estimates as well as the credibility intervals obtained for the parameters of the Gompertz model (Table 2) were consistent with the estimates obtained by Silva et al. (2023a) using the frequentist approach. Importantly, one of the significant advantages of working with the Bayesian methodology is obtaining the highest posterior density (HPD) interval, which is the interval with $(1 - \alpha)\%$ probability containing the most plausible values for the parameter (Guedes, Rossi, Martins, Janeiro, & Carneiro, 2014; Bolstad & Curran, 2016; Silva, Furtado, Frühauf, Muniz, & Fernandes, 2020).

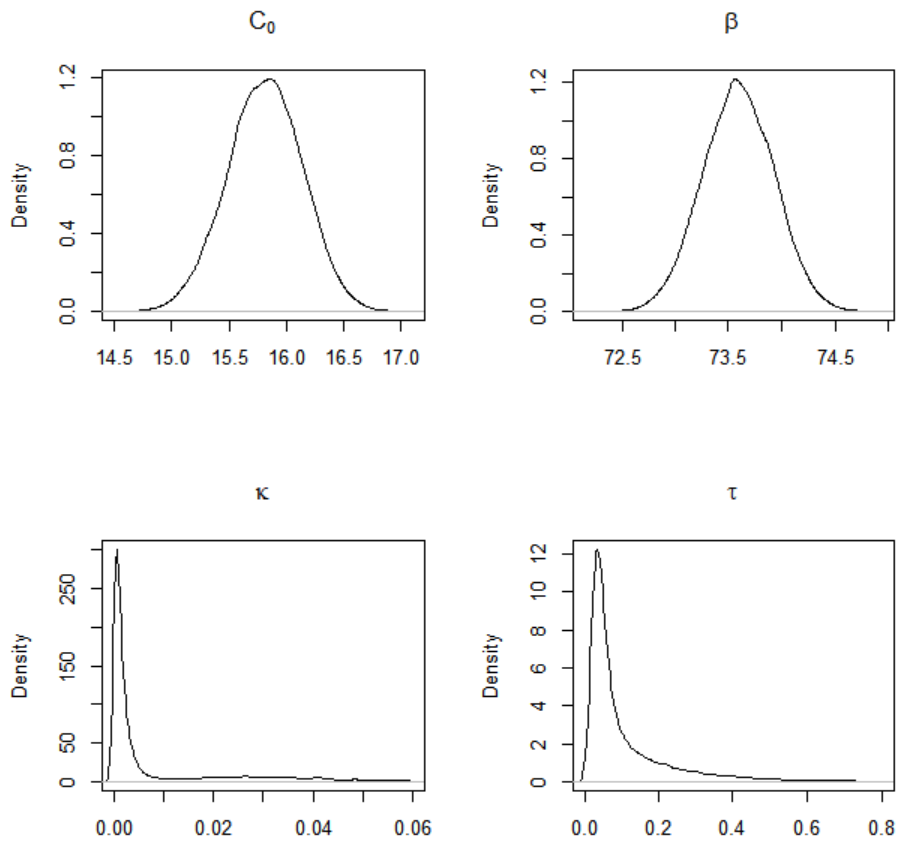


Figure 1. Posterior marginal distributions in soil carbon mineralization.

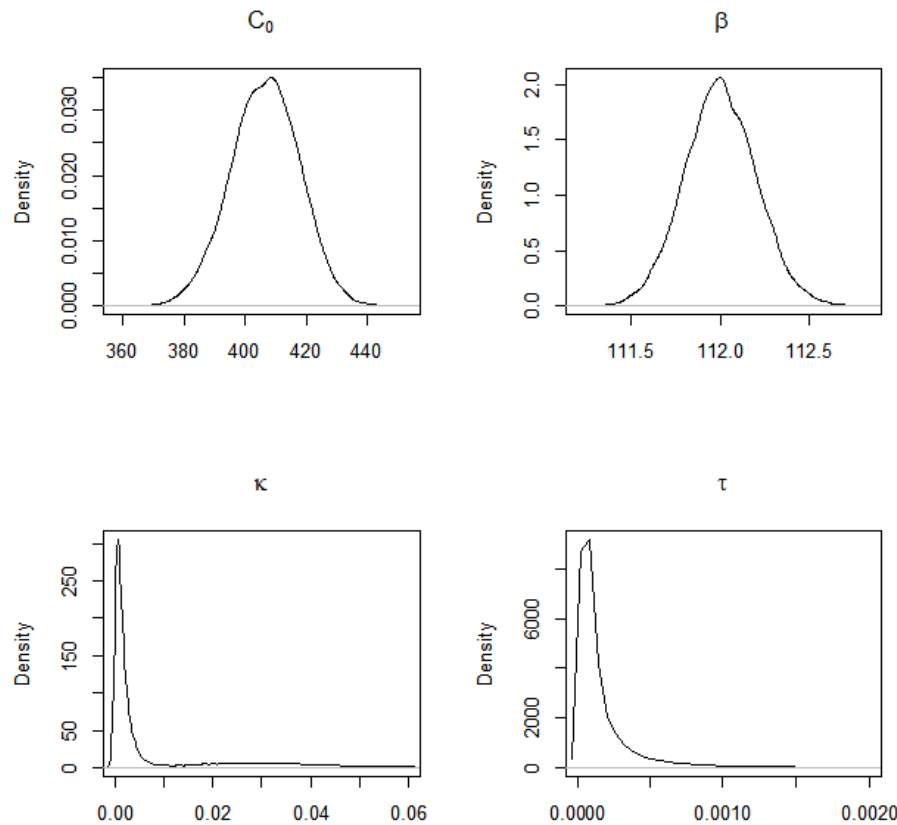


Figure 2. Posterior marginal distributions in carbon mineralization in soil with *S. atterimum*.

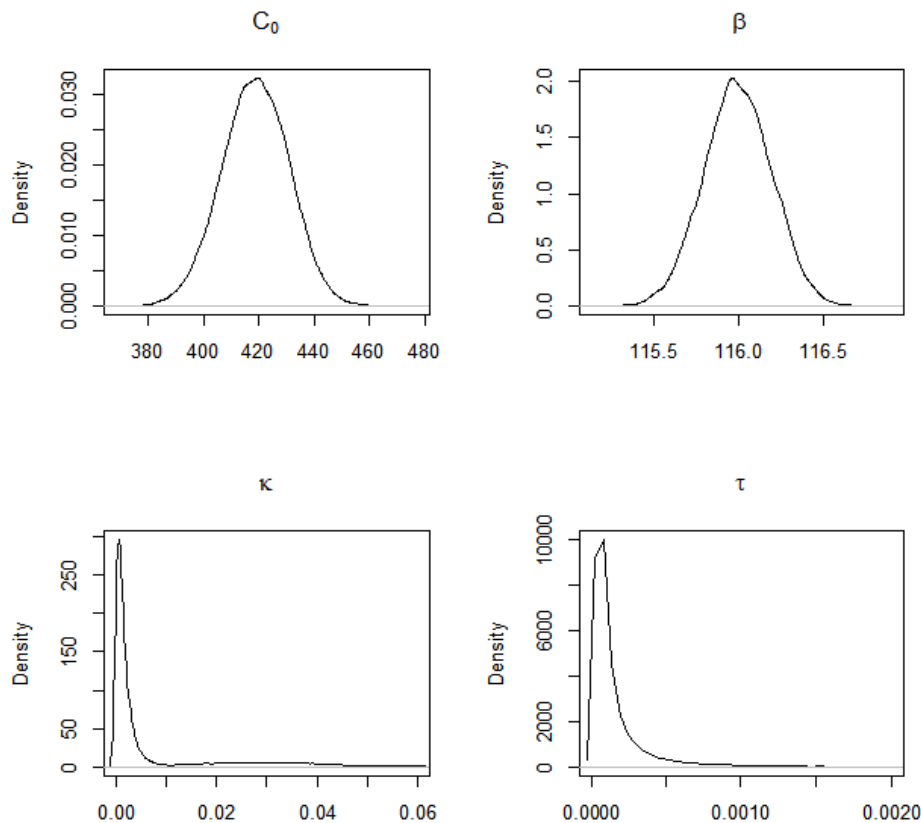


Figure 3. Posterior marginal distributions in soil carbon mineralization with *S. mucunoides*.

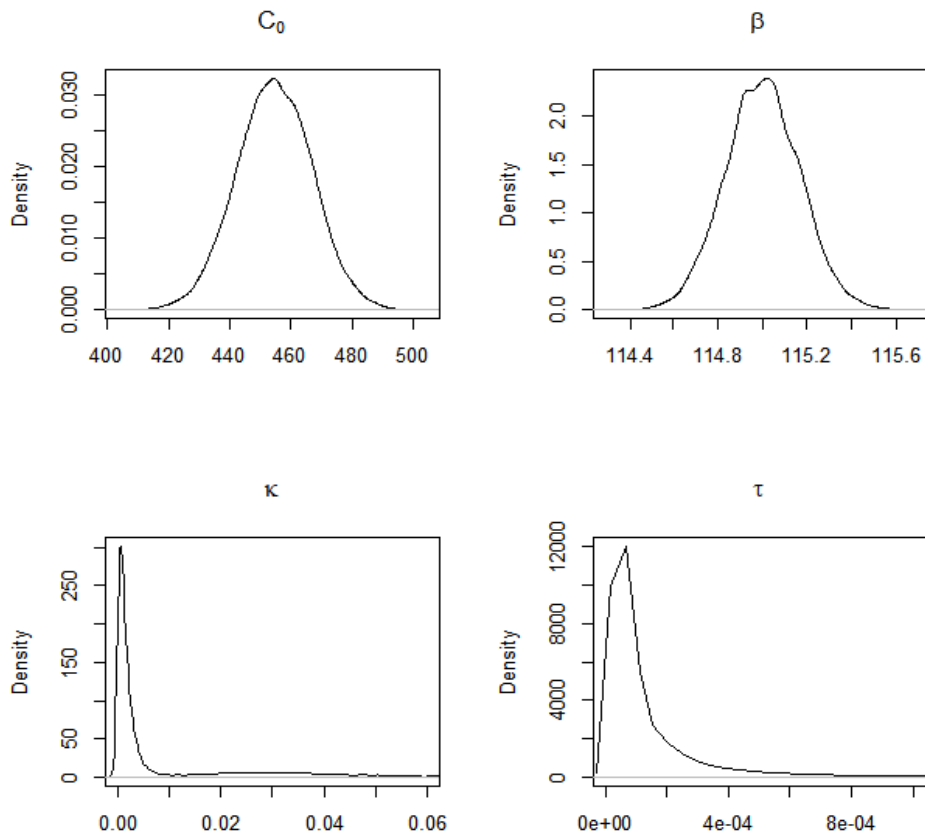


Figure 4. Posterior marginal distributions in soil carbon mineralization with *S. guianensis*.

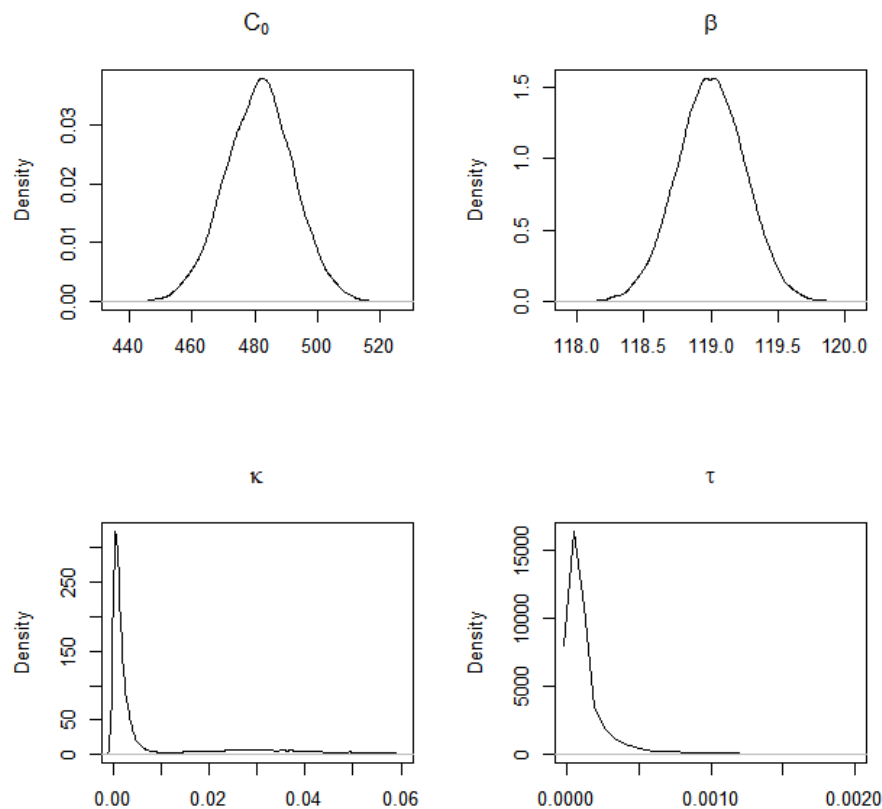


Figure 5. Posterior marginal distributions in soil carbon mineralization with *A. pinto*.

Conclusion

In the soil with legume addition, microorganisms took between 4 and 5 days to adapt until reaching the maximum decomposition rate. *A. pinto* showed a higher amount of potentially mineralizable carbon than the other treatments, with an average estimate of 481 mg CO₂. The treatments *S. atterrimum*, *S. mucunoides*, and *S. guianensis* had an average amount of potentially mineralizable carbon of 406, 418, and 454 mg CO₂, respectively, with this difference being statistically insignificant. Only soil had an average of 15 mg CO₂, which was statistically lower than the treatments where legumes were added to the soil.

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