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Nonlinear models to describe the growth of Jatropha plant (*Jatropha curcas* L.)[1]

Modelos não lineares para descrição do crescimento da planta de pinhão manso (*Jatropha curcas* L.)

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ABSTRACT - Brazil stands out in the renewable energy sector due to the growing demand for clean energy sources, mainly with biodiesel production, which uses vegetable oils and animal fats as raw material. With this, research has been developed with oilseed plants for this purpose and, among these plants, Jatropha has stood out for its productivity and ability to grow in regions with water scarcity. Thus, it is necessary to study the growth of this plant over time to assist management techniques and detection of factors that affect the plant development. Therefore, modeling this type of growth can subsidize knowledge and application of efficient techniques for agricultural practices. The objective of this study was to fit and compare the nonlinear Logistic and Gompertz models with four parameters in the description of growth in height of the Jatropha plant according to days after the phenological cycle in the second year of the plant development, totaling 25 observations. The models were fit using the statistical software R, considering the first order autoregressive error structure for the CNPAE-169 and CNPAE-259 accessions. All models fit well to the data from the three accessions under study, but the Logistic model stood out for the CNPAE-169 and CNPAE-102 accessions and the Gompertz model for the CNPAE-259 accession. The CNPAE-102 accession stood out from the others, presenting greater height in the study period.

Key words: Biodiesel. Growth curve. Renewable energy. Logistic. Gompertz.

RESUMO - A crescente demanda por fontes de energias renováveis, também conhecidas como energias limpas, faz com que o Brasil se destaque nesse setor, principalmente com a produção de biodiesel, o qual tem como matérias-primas óleos vegetais e gorduras de origem animal. Com isso, tem se desenvolvido pesquisas com plantas oleaginosas para este fim e, dentre estas plantas, o pinhão manso tem se destacado pela sua produtividade e capacidade de se desenvolver em regiões com escassez hídrica. Sendo assim, faz-se necessário o estudo do crescimento dessa planta ao longo do tempo para auxiliar nas técnicas de manejo e detecção de fatores que afetem o desenvolvimento da planta. Logo, a modelagem desse tipo de crescimento pode subsidiar o conhecimento e a aplicação de técnicas eficientes para as práticas agrícolas. Desta forma, o objetivo deste estudo foi ajustar e comparar os modelos não lineares Logístico e Gompertz com quatro parâmetros na descrição do crescimento em altura da planta de pinhão manso em função dos dias após o ciclo fenológico no segundo ano do desenvolvimento da planta, totalizando 25 observações. O ajuste dos modelos foi realizado através do software estatístico R, considerando-se a estrutura de erros autorregressivos de primeira ordem para os acessos CNPAE-169 e CNPAE-259. Todos os modelos aderiram bem aos dados dos três acessos em estudo, porém o modelo Logístico se destacou para os acessos CNPAE-169 e CNPAE-102 e o modelo Gompertz para o acesso CNPAE-259. O acesso CNPAE-102 se sobressaiu aos demais apresentando maior altura no período estudado.

Palavras-chave: Biodiesel. Curva de Crescimento. Energias Renováveis. Logístico. Gompertz.

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INTRODUCTION

The growing concern with environmental impacts has increased the global demand for clean, renewable and sustainable energy sources, making it possible to reduce the use of fossil fuels and placing biofuels at the center of attention and interest as a great alternative. Brazil has stood out in this context, due to its extensive experience in the generation and use of this energy source (AZEVEDO; LIMA, 2016; FREITAS *et al*., 2011; PADILHA *et al*., 2016).

The main raw materials for biodiesel production in Brazil are soybean, cotton and bovine fat, but jatropha (*Jatropha curcas* L.) has been standing out among the oilseed plants for this purpose, as well as presenting a high content of oil in seeds, has fast growth, resistance to long droughts, pests, diseases and also allows cultivation combined with other crops of food and economic interest (FIGUEIREDO *et al*., 2018; NÁPOLES *et al*., 2017; PADILHA *et al*., 2016).

However, according to Tomaz *et al*. (2020), breeding programs for *Jatropha curcas* are still scarce when compared to other oilseeds such as soybeans, peanuts and sunflowers. Therefore, it is necessary to investigate its agronomic aspects to better define cultivars, which can be done with the aid of non-linear models, as according to Jane *et al*. (2020a), these models have a sigmoidal nature, which better describes plant growth, being also more parsimonious and presenting estimates that generally have practical interpretations.

Several authors have found satisfactory results when using these models to describe plant and fruit growth (JANE *et al*., 2019, 2020b; MUIANGA *et al*., 2016; PRADO *et al*., 2020; RIBEIRO *et al*., 2018a, 2018b; SILVA *et al*., 2020). Among the most used nonlinear models for growth analysis, the Logistic and the Gompertz models with three parameters stand out, which have the lower horizontal asymptote set at zero (FERNANDES *et al*., 2015). However, in practice, there are cases in which this situation does not occur, and it is necessary to add an intercept parameter to the model, because with four parameters the model allows changing the lower horizontal asymptote and its parameters remain biologically interpretable.

Given the above, this study aimed to model the growth in height of three morphologically distinct Jatropha accessions as a function of the days after the beginning of the phenological cycle through the nonlinear Logistic and Gompertz models with four parameters.

MATERIAL AND METHODS

To fit the models, data from Gurgel *et al*. (2011), referring to the heights obtained from the second year of development of three morphologically distinct accessions of Jatropha: CNPAE-102 (toxic, susceptible to powdery mildew), CNPAE-169 (non-toxic, susceptible to powdery mildew) and CNPAE-259 (toxic, resistant to powdery mildew). According to the authors, accessions with undetectable levels of phorbol ester in grains were considered non-toxic.

For the experiment, accessions were obtained from the Jatropha germplasm bank installed in the experimental area of Embrapa Cerrados in Planaltina, Distrito Federal, Brazil. According to the Köppen-Geiger climate classification, the local climate is Aw, tropical with rainy summer and dry winter. The total rainfall in the period studied was 1,089.4 mm with a maximum temperature of 28.5 ºC and a minimum of 17 ºC. The soil is classified as Red Latosol with high clay content.

Plant height was measured every two weeks from the base of the trunk to the top of the tallest branch in a period of one year, starting on August 21, 2009 (day 1) and ending on July 16, 2010 (day 337), totaling 25 observations. Logistic (Eq. 1) and Gompertz (Eq. 2) nonlinear models with four parameters were used to analyze plant height as a function of days after the onset of the phenological cycle.

$$Y_i = \alpha_0 + \frac{\alpha_1}{1 + e^{-\kappa(x_i - \beta)}} + u_i \quad (1)$$

$$Y_i = \alpha_0 + \alpha_1 e^{-e-\kappa(x_i - \beta)} + u_i \quad (2)$$

In the equations above, Y_i represents the i-th observed height value in m, with i = 1,2,..., n, n is the number of times in which the measurements were taken; x_i refers to the time at i-th measurement, given in days, after the onset of the phenological cycle; α_0 is the starting point of growth under study; α_1 is the increase in height achieved by Jatropha; β is the abscissa of the inflection point, that is, where plant growth slows down, stabilizing at its maximum value; κ is the maturity index and u_i is the fit residual at i-th measurement described by (Eq. 3):

$$u_i = \phi_1 u_{(i-1)} + \ldots + \phi_p u_{(i-p)} + \varepsilon_i \quad (3)$$

In equation 3, ϕ_1 is the first-order autoregressive parameter; $u_{(i-1)}$ is the fit residual in the time prior to the i-th measurement; ϕ_p is the p-th order autoregressive parameter; $u_{(i-p)}$ is the fit residual in p time prior to the i-th measurement; ε_i is the white noise with normal distribution, zero mean and constant variance, $\varepsilon_i \sim N(0,\sigma^2)$. For the case of independent errors, the ϕ_i parameters will be null, so it follows that $u_i = \varepsilon_i$ (MUIANGA *et al*., 2016; RIBEIRO *et al*., 2018b; SOUZA *et al*., 2014).

Parameters were estimated using the least squares method, which consists of minimizing the sum of the square of the residuals, thus generating a system of normal equations. However, for nonlinear models, this system does not have an explicit solution, requiring the use of iterative methods to find an approximate solution (FERNANDES; PEREIRA; MUNIZ, 2017). In this study, the Gauss-Newton algorithm was used as an iterative method and the choice of initial values to be used for the execution of the iterative process was performed based on an initial exploratory analysis of the data. The significance of parameter estimates was verified by Student's t-test and the confidence interval was calculated at the 99% confidence level.

According to Muniz, Nascimento and Fernandes (2017), the inflection point coordinates of each model can be obtained with three parameters based on the parameter estimates, in which $\hat{\beta}$ is the abscissa for both models and the ordinate is given by $\tilde{\alpha}/2$ and $\tilde{\alpha}/e$ for the Logistic and Gompertz models, respectively, where e is the Euler number ($e \approx 2{,}718$) and $\tilde{\alpha}$ is the upper horizontal asymptote of the models, which is given by $\tilde{\alpha} = \tilde{\alpha}_0 + \tilde{\alpha}_1$. In parameterizations with four parameters, it is observed that $\hat{\beta}$ remains the abscissa for both models and the ordinate is given by $\tilde{\alpha}_0+(\tilde{\alpha}_1*0{,}5)$ and $\tilde{\alpha}_0+(\tilde{\alpha}_1*0{,}37)$ for the Logistic and Gompertz models, respectively, which corroborates Jane *et al*. (2019), who observed that the inflection point of the Logistic and Gompertz models with four parameters occur above the inflection points of these same models with three parameters. Graphical analysis can also be performed using the first derivative of the functional forms of the fitted models, and it is possible to observe that at the inflection point, the first derivative reaches the maximum growth rate.

The inflection point of the curve is important for the researcher, because it allows to define the moment when the growth of the study object starts to slow down, that is, the instantaneous growth rate changes from increasing to decreasing.

After fitting the models, the assumptions of normality, homoscedasticity and independence of the residual vector were checked by the Shapiro-Wilk, Breusch-Pagan and Durbin-Watson tests, respectively, at the 1% level of significance, as well as through the analysis of the graphic distribution of residuals. According to Fernandes *et al.* (2014), this is a very important step in modeling, because if there is a violation of any of these assumptions, the model is not adequate to describe the phenomenon under study.

Goodness-of-fit of the models to the data was based on the results found for the adjusted coefficient of determination (Eq. 4), the residual standard deviation (Eq. 5) and the corrected Akaike information criterion (Eq. 6):

$$R^2aj = 1 - \frac{(1-R^2)(n-i)}{(n-p)} \quad (4)$$

$$DPR = \sqrt{QME} \quad (5)$$

$$AIC_C = n1n\left(\frac{SQR}{n}\right) + \frac{2p(p+1)}{n-p-1} \quad (6)$$

where, R^2 = 1- (SQR/SQT) is the coefficient of determination that indicates the variation in data explained by the model; SQR is the sum of squares of the residuals; SQT is the total sum of squares; n is the number of observations; p is the number of parameters of the fitted models; i is related to the fit of the intercept on the curve, being equal to 1 if there is an intercept and 0 otherwise and QME is the mean square of the error. The model with greater adherence to the data is the one with the lowest values for DPR and AIC_C and the highest value for R^2_{aj}.

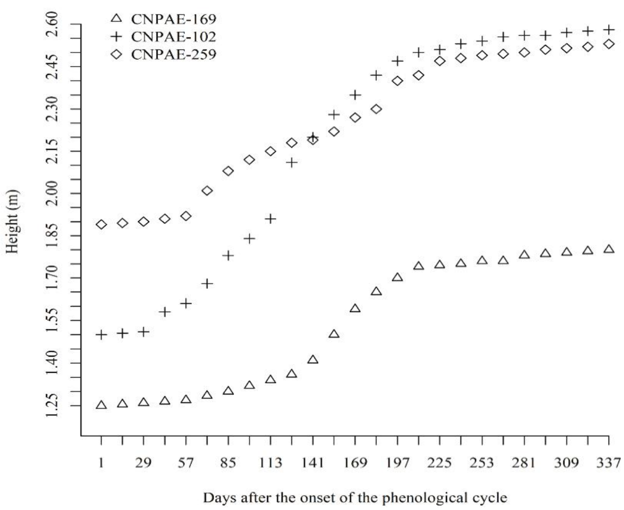
For fitting and comparing models and all the computational part of this work, the R statistical software (R CORE TEAM, 2020), with open access, was used, using the packages "*car*", "*lmtest*", "*nlme*" and "*qpcR*".

RESULTS AND DISCUSSION

In Figure 1, a sigmoidal behavior of plant height growth can be observed in relation to days after the onset of the phenological cycle, with an indication for the use of a non-linear model. It is possible to observe an upper and a lower asymptotes, suggesting the use of nonlinear models with four parameters, corroborating Paine *et al.* (2012), who described the behavior of the four-parameter model in their studies with plant growth, obtaining a graphical representation similar to that found in Figure 1.

After fitting the Logistic and Gompertz models with four parameters to the height data as a function of the days after the onset of the phenological cycle, a residual analysis was performed. Table 1 lists the results obtained for the

Figure 1 – Graphic representation of plant height growth of accessions CNPAE-169, CNPAE-102 and CNPAE-259 in relation to days after the onset of the phenological cycle



Shapiro-Wilk, Bresch-Pagan and Durbin-Watson tests for the residuals of the models. Results of the Shapiro-Wilk and Breusch-Pagan tests indicated that the assumptions of normality and homogeneity of variances, respectively, were met at the 1% level of significance (p-value > 0.01) for the three accessions. Durbin-Watson test evidenced that the assumption of residual independence was met for the CNPAE-102 accession. Similar results were reported by Jane *et al*. (2019) and Lúcio *et al.* (2016) in studies of pepper growth and cherry tomato production, respectively, reporting independence of the residual vector.

For the CNPAE-169 and CNPAE-259 accessions, the Durbin-Watson test showed residual autocorrelation (p-value < 0.01), indicating dependence between the height measurements of the plants along the phenological cycle in these accessions. Ribeiro *et al.* (2018b) demonstrated the importance of modeling this autocorrelation and including it in the model to ensure greater precision in the estimates. Muniz, Nascimento and Fernandes (2017) verified that the incorporation of the autocorrelation parameter (AR1) reduced the residual standard deviation, providing more reliable estimates of parameters of the Logistic and Gompertz models, in the study on cocoa fruit growth. Similar results were reported by Frühauf *et al.* (2020), Jane *et al.* (2020a) and Silva *et al.* (2020), who also observed self-correlated errors in their studies of fits to nonlinear models in describing the growth of cedar trees (*Cedrela fissilis*), sugarcane varieties and blackberry fruits, respectively.

In Figures 2, 3 and 4, it is possible to observe the graphic distribution of the residual vector for the Logistic and Gompertz models with the incorporation of the autoregressive parameter (AR1) for the height data of Jatropha plants for the studied accessions. Graphs of residuals versus the adjusted values (Figures 2(A, C), 3(A, C) and 4(A, C)) were used as a graphical analysis to check the residual assumptions, through which one can detect heteroscedasticity, in addition to indicating a linear relationship between the explanatory variable and the response variable through some trend in the points.

The normal quantile-quantile plot (Figures 2(B, D), 3(B, D) and 4(B, D)) is used to detect residual non-normality, whereas in Figures 2(D), 3(D) and 4(D), a slight asymmetry was observed, but not detected in the Shapiro-Wilk tests.

Table 2 presents the parameter estimates and their respective 99% confidence intervals, based on fitting the Logistic and Gompertz models for plant height measurements of three jatropha accessions. The structure of first-order autoregressive errors for CNPAE-160 and CNPAE-259 accessions was considered. All estimated parameters were significant, by the t-test, at the 1% level of significance.

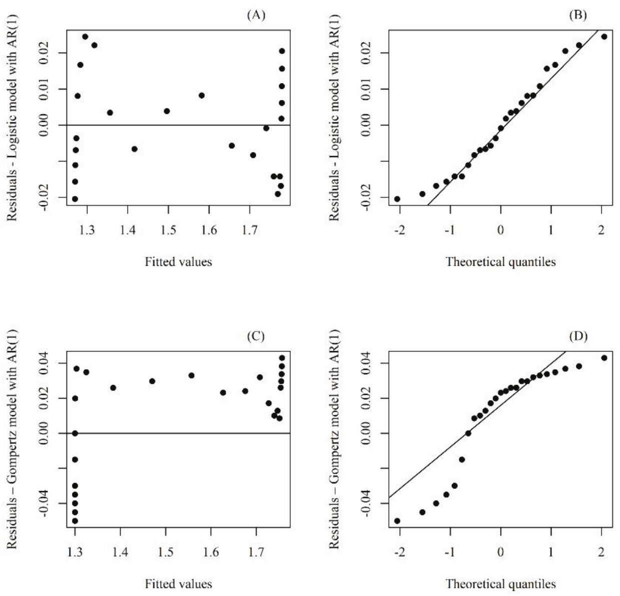
Considering the results in Table 2, one can observe the non-nullity of the parameters due to the non-inclusion of zero in their confidence intervals, which indicates a possible significance for their estimation. It is also possible to notice a distinct growth in each of the accessions, as the CNPAE-169 access showed less growth in the study period, with an increase of 0.509 m (Logistic) and 0.457 m (Gompertz), reaching an asymptotic height of 1.779 m (Logistic) and 1.757 m (Gompertz) at the end of the phenological cycle. The accession CNPAE-102 showed the greatest growth over the study period, with an

Table 1 – P-value for the Shapiro-Wilk, Breusch-Pagan and Durbin-Watson tests used in the residual vector analysis for fitting the Logistic (L) and Gompertz (G) models to the height of jatropha plants as a function of days after the phenological cycle

Accessions	Model	Shapiro-Wilk	Breusch-Pagan	Durbin-Watson
CNPAE-169	L	0.289	0.196	< 0.001*
	G	0.898	0.070	< 0.001*
CNPAE-102	L	0.034	0.037	0.455
	G	0.012	0.134	0.016
CNPAE-259	L	0.558	0.037	< 0.001*
	G	0.442	0.029	< 0.001*

* significant at the 1% probability level

Figure 2 – Graphic distribution of residuals for height of accession CNPAE-169, where (A) and (C) represent the fitted values in relation to the residuals and (B) and (D) represent the residual values in relation to the theoretical quantiles for the Logistic and Gompertz models with AR1



increase of 1.113 m (Logistic) and 1.073 m (Gompertz) and asymptotic height 2.570 m (Logistic) and 2.591 m (Gompertz). The CNPAE-259 accession showed an intermediate growth behavior, reaching 2.554 m (Logistic) and 2.576 m (Gompertz) of asymptotic height and increment of 0.741 m (Logistic) and 0.702 m (Gompertz).

Figure 3 – Graphic distribution of residuals for the height of accession CNPAE-102, where (A) and (C) represent the fitted values in relation to the residuals and (B) and (D) represent the residual values in relation to the theoretical quantiles for the Logistic and Gompertz models

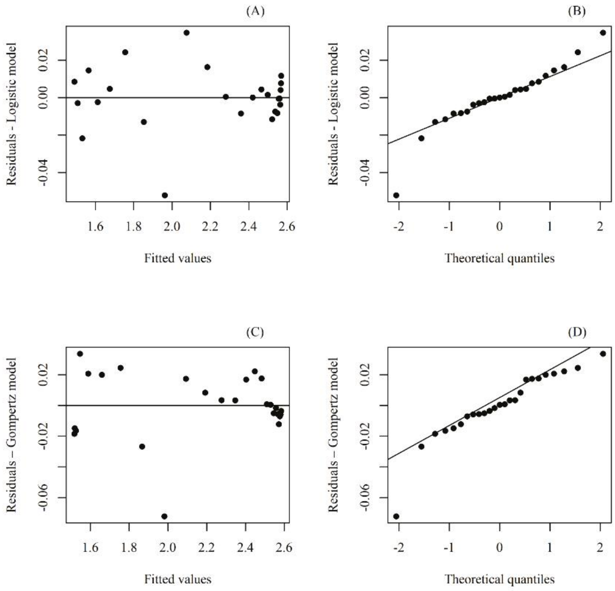


Figure 4 – Graphic distribution of residuals for the height of accession CNPAE-259, where (A) and (C) represent the fitted values in relation to the residuals and (B) and (D) represent the residual values in relation to the theoretical quantiles for the Logistic and Gompertz models with AR1

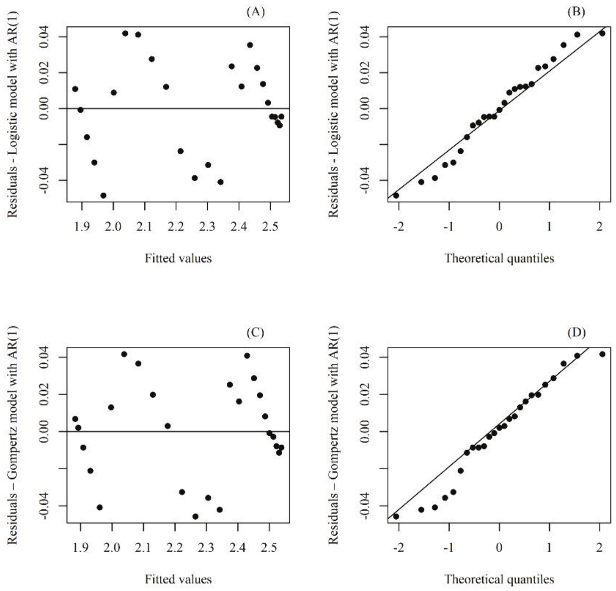


Table 2 – Estimates and upper limit (UL) and lower limit (LL) parameters for fitting Logistic and Gompertz models to the height of Jatropha plants considering first-order autoregressive errors for CNPAE-169 and CNPAE-259 accessions

Accessions	Parameters	Logistic			Gompertz		
		LL	Estimate	UL	LL	Estimate	UL
CNPAE-169	$\tilde{\alpha}_0$	1.234	1.270	1.307	1.214	1.300	1.386
	$\tilde{\alpha}_1$	0.459	0.509	0.560	0.389	0.457	0.526
	β	152.912	159.663	166.414	149.695	154.694	159.693
	κ	0.038	0.049	0.059	0.031	0.038	0.046
	$ø_1$	0.183	0.810	0.969	0.711	0.972	0.998
CNPAE-102	$\hat{a}_0$	1.425	1.457	1.487	1.489	1.518	1.546
	$\tilde{\alpha}_1$	1.076	1.113	1.153	1.035	1.073	1.115
	β	116.183	119.396	122.441	100.659	104.633	108.441
	κ	0.027	0.029	0.032	0.019	0.021	0.023
CNPAE-259	$\tilde{\alpha}_0$	1.691	1.813	1.934	1.803	1.874	1.945
	$\tilde{\alpha}_1$	0.575	0.741	0.907	0.577	0.702	0.827
	β	108.700	131.605	154.511	94.152	113.600	133.048
	κ	0.011	0.018	0.025	0.008	0.013	0.018
	$ø_1$	0.197	0.576	0.805	0.224	0.599	0.819

Gohil and Pandya (2009) observed similar results for height in different Jatropha genotypes and indicated that these growth parameters can be used to estimate the genetic heritability of the plant, which will ultimately contribute to the selection involved in plant breeding work.

The estimates found present satisfactory results, as according to Gurgel *et al.* (2011), the initial height of plants in the second year of development was 1.80m and Arruda *et al*. (2004) noticed that Jatropha has a fast growth, reaching a height of 2 to 3 m when adult and being able to reach up to 5 m under special conditions.

The results also corroborate those found by Santos *et al*. (2010), which showed that the phenology and growth of jatropha grown in *zona da mata*, in the state of Alagoas, presented an average height of 147 cm for plants from 6 to 21 months of age. Ginwal, Rawat and Srivastava (2004) and Rao *et al*. (2008) also observed similar results for height in different Jatropha genotypes.

According to Jane *et al.* (2020a), the inflection point (IP) is very important, as it indicates the date of greatest plant growth, after which growth begins to increase at decreasing rates until stabilization. Through the estimates found and Figures 5, 6 and 7, it is possible to observe the inflection point (IP) of the curves, which for the CNPAE-169 accession has the IP coordinates (159.66; 1.53) for the Logistic model and IP(154.69; 1.47) for the Gompertz model, indicating that the growth of Jatropha plant starts to be decelerated at approximately 150 days of the phenological cycle, for the CNPAE-102 accession, the IP coordinates (119.40; 2.01) for the Logistic model and IP(104.63; 1.91) for the Gompertz model, indicating a growth deceleration around 110 days of the phenological cycle and for the CNPAE-259 accession, the IP coordinates (131.61; 2.18) for the Logistic model and IP(113.60; 2.13) for the Gompertz model, growth decelerates at approximately 120 days of the phenological cycle.

Figure 5 – Growth rates in height of Jatropha plants of the CNPAE-169 accession obtained through the first derivative of the Logistic (A) and Gompertz (B) models where IP is the inflection point

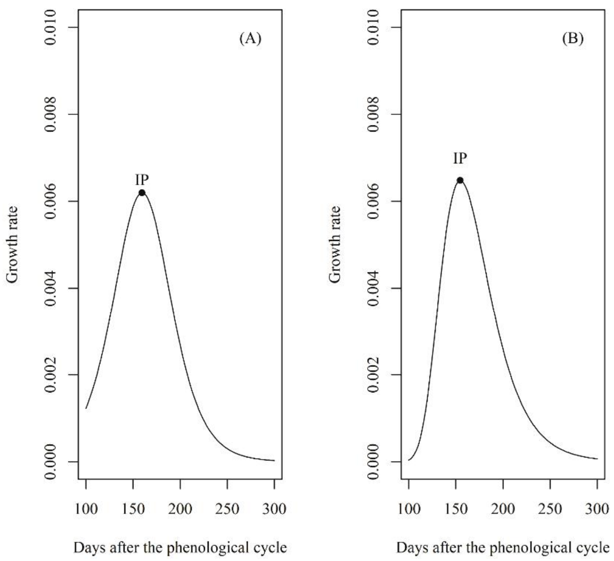


Figure 6 – Growth rates in height of Jatropha plants of the CNPAE-102 accession obtained through the first derivative of the Logistic (A) and Gompertz (B) models where IP is the inflection point

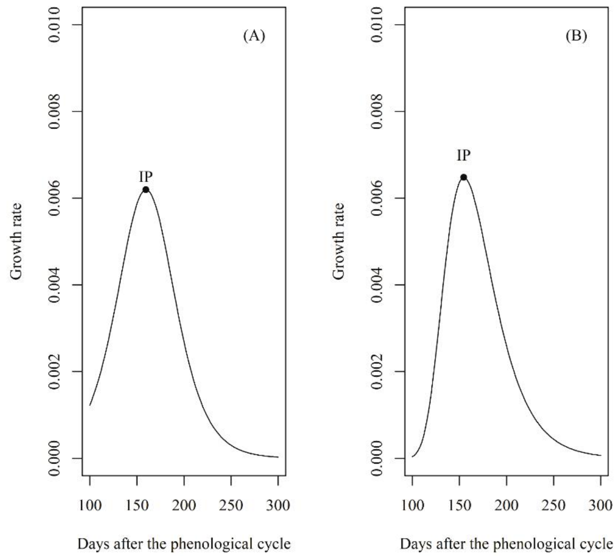


Figure 7 – Growth rates in height of Jatropha plants of the CNPAE-259 accession obtained through the first derivative of the Logistic (A) and Gompertz (B) models where IP is the inflection point

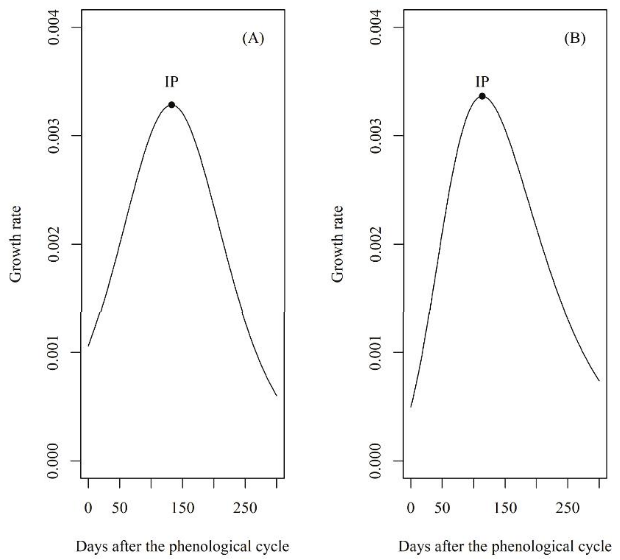


Table 3 – Criteria for evaluating the goodness-of-fit of Logistic and Gompertz models with first-order autoregressive error structure for CNPAE-169 and CNPAE-259 accessions

Accessions	Logistic			Gompertz		
	R^2_{aj}	DPR	AIC_C	R^2_{aj}	DPR	AIC_C
CNPAE-169	0.996	0.016	-152.611	0.971	0.044	-144.992
CNPAE-102	0.998	0.017	-124.252	0.997	0.023	-110.060
CNPAE-259	0.986	0.027	-109.963	0.986	0.027	-110.264

Figure 8 – Fitting the Logistic and Gompertz models to the height data of Jatropha plants from the CNPAE-169 accession with first-order autoregressive error structure (AR1)

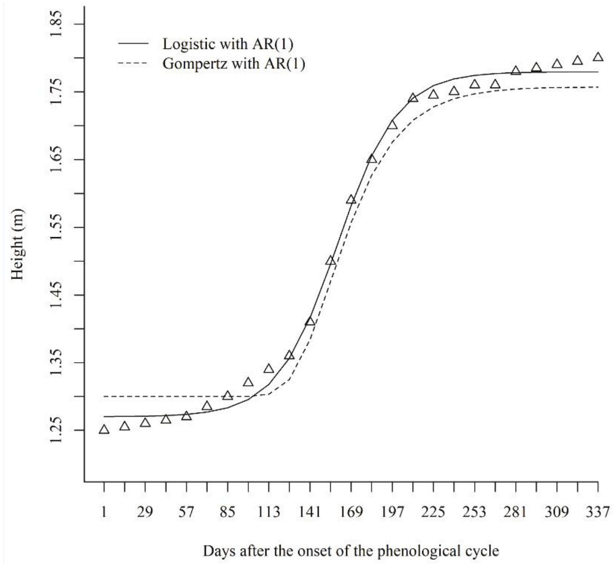


Figure 9 – Fitting the Logistic and Gompertz models to the height data of Jatropha plants from the CNPAE-102

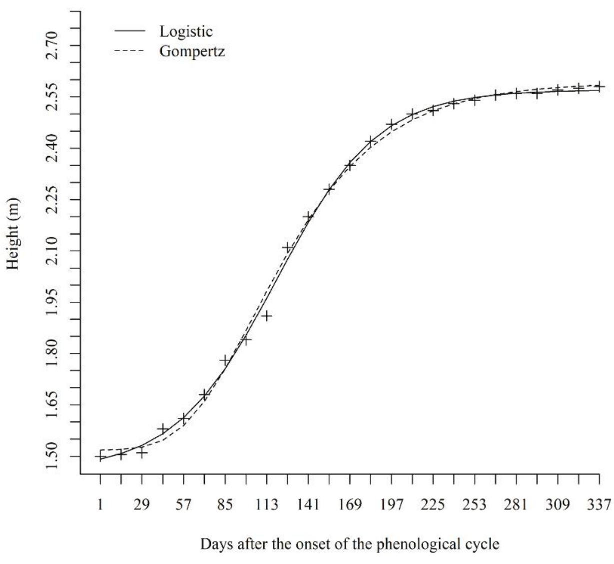
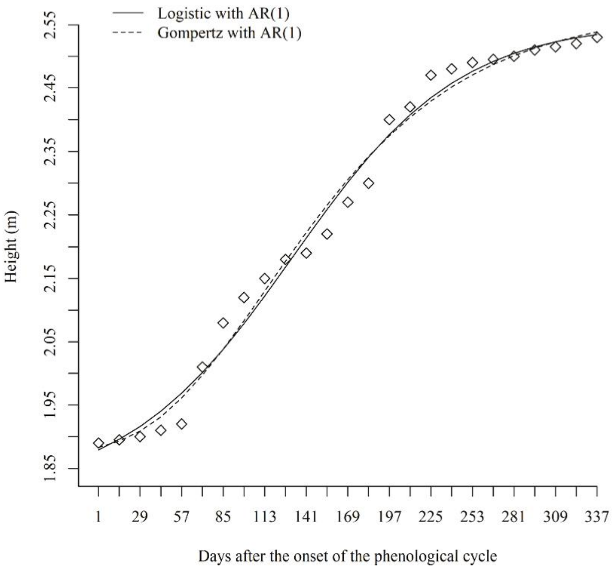


Figure 10 – Fitting the Logistic and Gompertz models to the height data of Jatropha plants from the CNPAE-259 accession with first-order autoregressive error structure (AR1)



The results obtained from the abscissa of the inflection point (β) are close to those found by Gurgel *et al*. (2011), who obtained 152 days for the CNPAE-169 access, 114 days for CNPAE-102 and 110 days for CNPAE-259 for the onset of growth deceleration. It can be seen that in the Gompertz model, the inflection point occurred a little before the Logistic model, as this model is not symmetrical around this point.

Table 3 shows the results of the criteria used to assess the goodness-of-fit, which indicate good fits for both models, however, the Logistic model presented a higher value of R^2_{aj} and lower values of AIC_C and DPR for accessions CNPAE-169 and CNPAE-102. Regarding the CNPAE-259 accession, the Gompertz model presented similar results for R^2_{aj} and DPR and a lower value for the AIC_C, indicating that it was the most suitable for this accession.

Figures 8, 9 and 10 illustrate the fits of the Logistic and Gompertz models considering the first-order autocorrelated error structure for the CNPAE-169 and CNPAE-259 accessions fitted for jatropha plant height along the phenological cycle. Visual analysis evidences a sigmoidal growth pattern in the data under study, with the presence of lower and higher asymptotes, and a good fit of the models to the data can be noticed.

In the present study, the nonlinear models with four parameters proved to be important for growth analysis, as it makes possible to know the plant behavior and make efficient decisions regarding agricultural practices and selection for breeding.

CONCLUSIONS

1. The three accessions of Jatropha plants in the second year of development presented a sigmoidal growth pattern characteristic of a model with four parameters, and were well described by the Logistic and Gompertz models;
2. The Logistic model obtained a good fit for the CNPAE-169 and CNPAE-102 accessions, while the Gompertz model for the CNPAE-259 accession;
3. The growth among accesses was distinct, in which the CNPAE-102 accession had the greatest growth, followed by CNPAE-259, and the CNPAE-169 accession had the smallest growth;
4. For accessions CNPAE-169 and CNPAE-259, residual autocorrelation was found for both models, indicating dependence between measurements of plant heights along the phenological cycle in these accessions, thus the first-order autoregressive error structure (AR1) was considered to correct this assumption deviation.

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