British Journal of Research

www.britishjr.org

Original Article

Polynomial Modelling of Allelopathic Effect of Topsoil Extract

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ABSTRACT

Objective: This paper seeks to model the allelopathic effect of topsoil extract transferred from Tectona grandis L. plantation on *lycopersicum esculentum* seed germination and seedling growth
Research Methods: A mathematical model will be formulated using polynomial regression based on the data collected. This model was used instead of other proposed models because the relationship between the two variables was curvilinear. Cubic spline method was used to smooth the model to avoid oscillations between exact fit values. Computer program MATLAB was used in the analysis of the data.
Results: It was found that the quartic polynomial regression model was the best fitted model for the collected data with least square parameters estimates given by $P = 99.1892 + 7.9280CL - 13.4785CL^2 + 2.7142CL^3 - 0.1782CL^4$
Conclusion: This study has demonstrated that the allelopathic effects present in transferred topsoil samples of *T. grandis* on *lycopersicum esculentum* seed germination can be modeled using the quartic polynomial model for any concentration of topsoil between 0 kg and 7 kg.

Keywords: Multiple regression model, Polynomial regression modeling, Root mean squared error, *R*-squared, Allelopathy, Topsoil extracts.

INTRODUCTION

Allelopathy is a natural phenomenon whereby one plant releases a substance which has inhibitory and stimulatory effects on other plants and micro organisms sharing the same habitat [1,2]. A large number of plants have been identified as being allelopathic, and one of which is *Tectona grandis Linn* (Teak). The soil supporting the growth of teak have been found to contain maximum levels of exchangeable calcium and potassium [3,4] the absence of which can result in restricted growth of roots, stems, leaves and many other parts of the plant [5]. Allelopathic chemicals found in teak can be present in any part of the plant in addition to the surrounding soil. Recently, the allelopathic influence of leaf extracts on some plants has been reported [6,7,8]. Extracts from the seed and bark have also been used as antifeedant, larvicidal and growth inhibitors [9,10]. Extensive study has also showed that the presence of allelopathy is mainly demonstrated through symptoms such as plant damage, low germination, growth or development; presence of substances or organisms (plants or microbes) which contain or have the ability to produce phytotoxic chemicals in the vicinity of affected plants; the presence of phytotoxic chemicals in the plants or extract soils in the vicinity of affected plants [11]. The source of allelopathic compounds especially in soils has been traced to leaching, root exudation, microbial decomposition and enzymatic degradation of allelopathic plant material [1]. Most allelochemicals are classified as secondary metabolites of the plant [12] and once they are dispatched in the soil, they enter the complex plant - soil system where diverse factors act on their accumulation, availability and eventually their effective influence on target plants. It is to investigate further the transferability of concentration dependent stimulatory or inhibitory effect of allelochemical - laden extract of top soil from teak plantation that this research was conducted [13,14]. Ref [14] investigated the allelopathic effects present in transferred topsoil extracts of *T. grandis* on *lycopersicum esculentum* seed germination and growth of the seedling. The allelopathic influence increased with increasing mass of topsoil sample used.

Mathematical modelling is making increasingly significant contributions among the disciplines involved in allelopathy research. The fundamentals of allelopathy were expounded by An *et al* [18], following from that the authors in [19] studied plant residue alleopathy. Separating allelopathy from competition, characterizing allelopathy and its ecological roles and the modeling of allelopathy effects by external factors, like density of target plants have recently been studied in [15,16,17,26]. The use of nonlinear regression models like log-logistic in allelopathy modeling has been introduced by Belz *et al* in [27].

In the study of allelopathy, biological responses to allelochemical are frequently expressed as percent of control. With the control set at 100% it is, therefore hypothesized that the biological response to allelochemical, P% of control, is mathematically expressed by the following model:

$$P = 100 + S - I \qquad (1)$$

Where P represents the biological response to an allelochemical, S and I are biological responses to the stimulatory and inhibitory attributes of the allelochemical respectively, and are expressed in the model by enzyme kinetics [18]. This model has provided the platform for the analysis of experimental data, prediction of allelopathic effects on plants and for theoretical exploration of "fundamentals of allelopathy matters" [15]

In this work polynomial modeling will be used to interpolate the influence of allelopathy of top soil of *T. grandis* on *lycopersicum esculentum* seed germination or seedling growth, the curvilinear relationship between the two variables of the data collected as seen in Figure1 is the basis for the use of this model. Polynomials are mostly used in modeling a nonlinear relationship between a response variable and an explanatory variable. Polynomials are "useful for interpolation, but notoriously poor at extrapolation". [20]. In this research we do not intend to extrapolate but the model could be use minimally for extrapolation purposes.

MATERIALS AND METHODS

Location of the experiment

The experiment was carried out at the Crops and Soil Science Department farm, College of Agriculture Education, University of Education, Winneba, Mampong - Ashanti (Longitude 0.05° and 1.30° W and Latitude 6.55° and 7.30° N), in August, 2014. The soil at the farm was largely sandy loam.

Land and sample preparation

A plot of land measuring 20m by 30m was prepared and divided into fifteen mini - plots each with three sections for the study. Fourteen of the mini - plots were selected for the treatments and the remaining was the control and respectively labelled from A to O. Topsoil samples were collected from a teak plantation, crushed into fine powder and weighed into 0.5kg, 1kg, 1.5kg, 2.0kg, 2.5kg, 3.0kg, 3.5kg, 4.0kg, 4.5kg, 5.0kg, 5.5kg, 6.0kg, 6.5kg and 7.0kg packs. The seeds of a local variety of tomato (Power Rano) were obtained from a certified seed supplier.

Treatment with the topsoil samples

Starting with the mini - plot marked A, fifty (50) tomato seeds were sown on each of the three sections after which 0.5 kg of topsoil sample was spread fully, by broadcasting, on each plot. The method was repeated using the remaining mini - plots B - N with respectively 1kg, 1.5kg, 2.0kg, 2.5kg, 3.0kg, 3.5kg, 4.0kg, 4.5kg, 5.0kg, 5.5kg, 6.0kg, 6.5kg and 7.0kg of the samples. Fifty (50) seeds were also planted on each sections of mini – plots, mini-plot O served as the control. The setup was then watered twice daily with water until the tomatoes fully germinated within 9 days.

THE MATHEMATICAL MODEL

The mathematical modeling will be formulated using polynomial regression based on the data collected from the results using the method in Ref [14]. All data will be solved and analyzed using MATLAB.

THE MODEL

A polynomial function of a scalar variable x is an expression of the form

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n \quad (2)$$

for some coefficients $a_0, a_1, \dots a_n$. If $a_n \neq 0$, then the polynomial is said to be of order *n*. A first-order polynomial equation is the equation of a straight line and a second-order polynomial equation also describes a parabola. Polynomials are just about the simplest mathematical functions that exist, requiring only multiplications and additions for their evaluation. Two polynomials are equal if they have the same coefficients of like powers of the variable.

A value $x = x_1$ such that $f(x) = 0$ is called the root of the polynomial function (2). Methods of getting the roots of a polynomial equation has been studied extensively in [21].

Polynomials are mostly used in modeling a nonlinear relationship between a response variable and an explanatory variable. Polynomials are "useful for interpolation, but notoriously poor at extrapolation".[20]. In this paper, we intend to use this model to interpolate the data points within [0, 7] as can be seen in Figure 1.

High order polynomial are seldom use in modeling because of parsimony and interpretability of the model but our interest in this research is to fit a polynomial that closely follows the pattern of the data and also provide accurate results and so higher order polynomials will be permitted if it provides a better fit to the data under study. The more complex a curve is, the more polynomials are needed to fully describe it. A polynomial of at most degree n is uniquely needed to fit $n+1$ distinct data points. [22]. Because there are the same number of coefficients in the polynomial as there are data points. This procedure of getting such a polynomial is justified by the use of the Lagrangian form of Higher polynomial in this result which is stated here without proof.

Theorem [22]
If $x_0, x_1, \dots, x_{n-1}, x_n$ are $n+1$ distinct points and $y_0, y_1, \dots, y_{n-1}, y_n$ are corresponding observations at these points, then there exists a unique polynomial $f(x)$, of at most degree n, with the property that

$y_k = f(x_k)$, for each $k = 0,1, \dots, n$

This polynomial is given by

$$f(x) = y_0 L_0(x) + \dots + y_n L_n(x) \qquad (3)$$

Where

$$L_k(x) = \frac{(x-x_0)(x-x_1)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)(x_k-x_1)\dots(x_k-x_{k-1})(x_k-x_{k+1})\dots(x_k-x_n)}$$

The polynomial (3) passes through each of the data points; the resultant sum of the absolute deviations is zero.

POLYNOMIAL REGRESSION MODEL

The k^{th} order Polynomial regression model in one variable can be expressed as

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \dots + \beta_k x^k + \epsilon \qquad (4)$$

Where k is the degree of the polynomial. This is a special case of a multiple regression with one independent variable. For example,

$$y = \beta_0 + \beta_1 x_1 + \beta_2 {x_1}^2 + \varepsilon \qquad (5)$$

is a quadratic polynomial model that provides a means of testing whether the relationship between y and x_1 is nonlinear(although the model itself is linear in the coefficients). A useful test for nonlinearities is provided by a standard t test of the null hypothesis that $\beta_2 = 0$ [23].

The mean squared error (MSE) is an unbiased estimator of the variance σ^2 of the random error term and is defined as

$$MSE = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-(k+1)} \qquad (6)$$

Where y_i are observed values, $\hat{y}_i$ are the fitted values of the dependent variable Y for the ith case and $n-(k+1)$ is the degree of freedom. The mean squared error is the average squared error, therefore the averaging is done by dividing by the $n-(k+1)$ degrees, MSE is a "measure of how well the regression fits the data" [24]. The root mean square error is given by the square root of the mean square error.

$$RMSE = \sqrt{MSE}.$$

The coefficient of determination (R-squared, R^2), of the regression equation is defined as

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \qquad (7)$$

Where $\bar{y}$ is the arithmetic mean of the y variable. R^2 is the proportion of the total variation in y explained by the regression of y on x. R^2 ranges in value between 0 and 1. An R^2 of 0 occurs when the regression model does nothing to help explain the variation in y. An R^2 of 1 may occur when all sample points lie on the estimated regression line. When R^2 value is 0.5 or below the regression explains only 50% or less of the variation in the data, therefore prediction may be poor.[23,24]

Following from (1.6) the adjusted R-squared is defined as

$$R^{*2} = R^2 - \frac{(1-R^2)k}{n-(k+1)} \qquad (8)$$

The adjusted $R-$squared is always smaller as the $R-$squared.

RESULTS AND DISCUSSION

Topsoil samples transferred from Teak plantation was used to explore similar effects and use that already exist in the leaf, bark and root extracts on germination and growth.

The addition of the samples of topsoil from the L. tectona grandis plantation affected the germination rate of the tomato seeds and this, from the results, mainly depended on the quantity(mass) of topsoil used for the treatment.[14] As can be seen from Table 1, as the quantity (mass) of topsoil samples increased, the percentage rate of germination of the tomato seeds decreased and therefore the allelopathic effect was strongest at the heaviest mass. The aim of this study was to model the allelochemical effect of the top soil sample from the Teak plant on the seed germination of lycopersicum *esculentum*. Since the simple scatter plot of the data from figure 1 gives a curvilinear relationship and our aim is to interpolate the data, polynomial model of the data will be appropriate in this direction. All analyses in the modeling process were done using a computer software, MATLAB and with its Curve Fitting Toolbox.

We fit a quadratic, cubic, quartic and a polynomial of degree 5, and see which of these models will provide a good approximation of the relationship as can seen in Figure 4

The basic statistical outputs are shown in Table 2. The quartic polynomial regression model is the best.The parameter estimates for this model are

$$P = 99.1892 + 7.9280CL - 13.4785CL^2 + 2.7142CL^3 - 0.1782CL^4 \qquad (9)$$

Where CL is the concentration levels of the allelochemical.

The cubic spline method was used to smooth the model as seen in Figure 2 and Figure 3. The smoothed quartic polynomial model is in a good agreement with a wide range of experimental data taken from the literature that has been modelled in Ref[18] suggesting that surface soil extract of *L.tectona grandis* inhibits or stimulates biological response in the germination of *lycopersicum esculentum.*

CONCLUSION

This study has demonstrated that the allelopathic effects present in transferred topsoil sampless of *L. Tectona grandis on the germination of lycopersicum esculentum* can be modeled using the quartic polynomial model for any concentration of topsoil between 0kg and 7 kg. This directly affects the seed germination and seedling growth of *lycopersicum esculentum.*

ACKNOWLEDGEMENT

The authors are very grateful to the reviewers for carefully reading the paper and for their comments and suggestions which helped to improve the paper.

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Table 1. Mean number of tomato seeds germinated and the germination percentage for various of treatments of topsoil extracts from teak plantation

Treatments (Concentration of Allelopathy)	Mean number of germinated seeds per section	*p %*
0.0	50	100
0.5	49	98
1.0	48	96
1.5	45	90
2.0	41	82
2.5	38	76
3.0	26	52
3.5	24	48
4.0	23	44
4.5	19	38
5.0	18	36
5.5	11	22
6.0	8	16
6.5	2	4
7.0	0	0

Table 2. Polynomial regression results

	Polynomial model			
	Quadratic	Cubic	Quartic	Degree 5
RMSE	5.3129	5.1860	4.4890	4.6005
R^2	0.9801	0.9826	0.9881	0.9888
R^{*2}	0.9767	0.9778	0.9834	0.9825

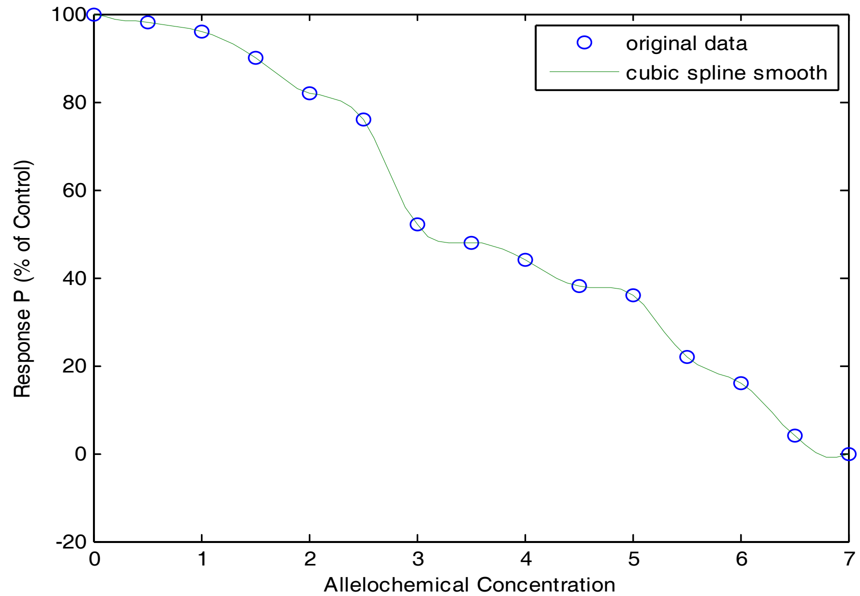

Figure 1. The variation of mean percentage germination with mass of topsoil extract

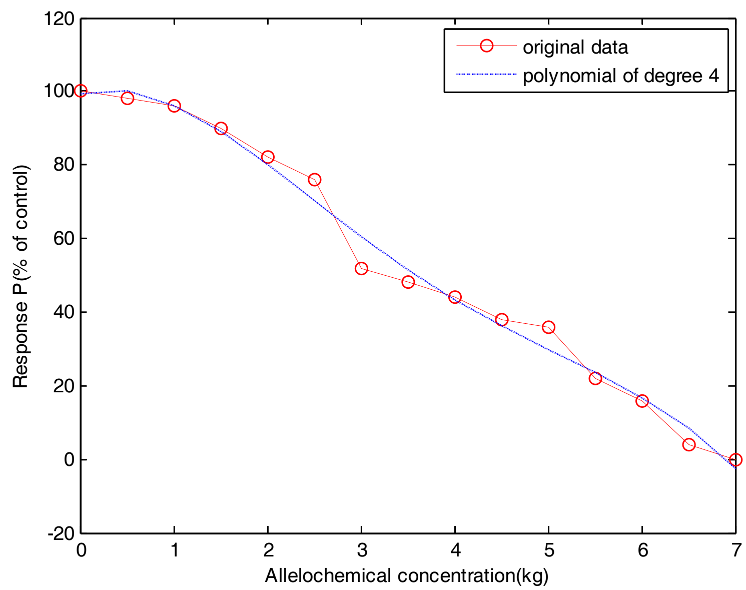

Figure 2. Comparison of polynomial model with measured data

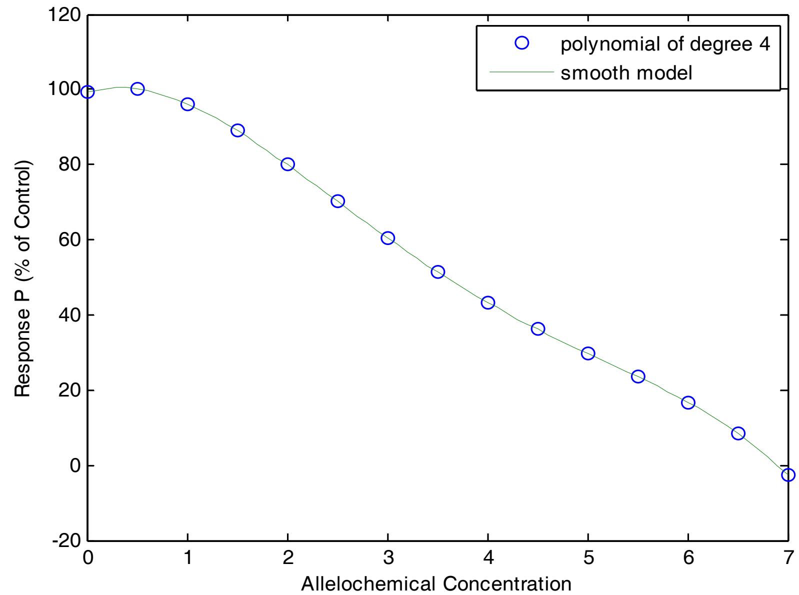

Figure 3. Fitted polynomial model with cubic spline smooth curve

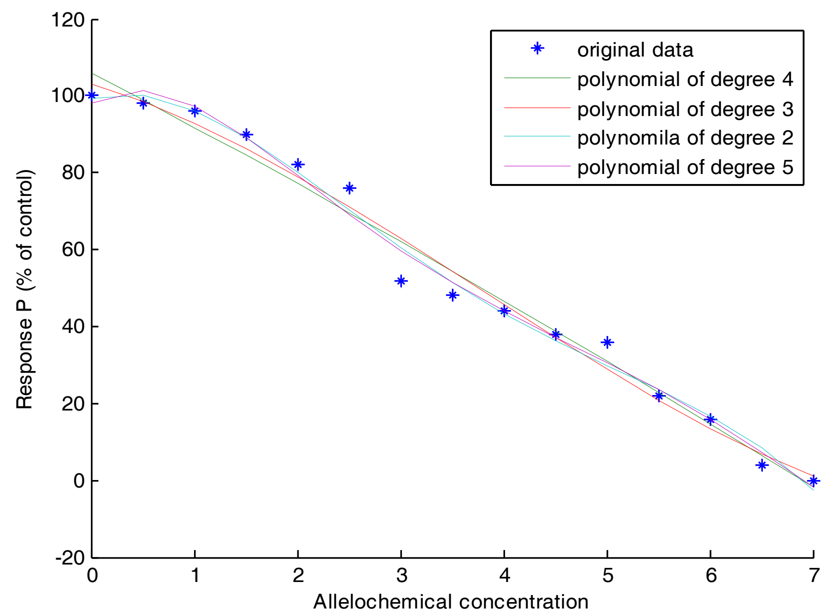

Figure 4. Comparison of polynomial models with measured data