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Study of Degradation Response of a Biopolymer Using Simple Regression Modelling

P. V. Hariganesh Sharma[1], R. Shobha[1*], C. Siddaraju[2] and T. S. Srivatsan[3]

[1]Department of Industrial Engineering and Management, Ramaiah Institute of Technology, Bangalore - 560054, Karnataka, India; shobar@msrit.edu

[2]Department of Mechanical Engineering, Ramaiah Institute of Technology, Bengaluru - 560054, India

[3]Department of Mechanical Engineering, The University of Akron, Akron, Ohio, USA

Abstract

Biodegradable polymer plastics have in recent years engendered considerable scientific interest due on account of their potential to be both technically viable and economically affordable alternatives to the family of conventional plastics due to aspects and intricacies specific to environmental concerns. Biodegradable polymers have in recent years provided much interest due on account of their degradability. The percentage degradation of the specific biopolymer that is chosen and used for a spectrum of performance-specific applications plays an important role in selecting the appropriate blend for the polymers chosen and used for the purpose of manufacturing. This research paper provides a cursory overview of the correct fit that is required for proper degradation of a biopolymer that can essentially be achieved by a polymer blend using simple linear regression analysis.

Keywords: *Biodegradable polymer, PLA-PBAT, Simple Linear Regression*

1.0 Introduction

The biodegradability of plastics is assessed using a simple linear regression model with a single explanatory variable, which conventionally in the Cartesian co-ordinates can be explained as the 'X' co-ordinate and the 'Y'co-ordinate. The sample points often consist of one independent variable and one dependent variable. In this research study, the variables are the following: (i) time as the independent variable, and (ii) degradation (%) as the dependent variable, which is carefully assessed using IBM SPSS as the tool. All of the details and intricacies specific to modelling were carried out using test data for both time and degradation of the chosen polymer blend (referred to henceforth through this manuscript as PLA-PBAT) that was obtained from an interim technical report of the company Biogreen biotech. The best fit for a sample of the chosen polymer blend (PLA-PBAT) was obtained by an analysis of the R value while concurrently studying the time that is required and essential for one hundred per cent [100%] degradation.

The references specific to the occurrence of degradation of a polymer, at the molecular level, have been studied under laboratory conditions[1]. This has helped in establishing an understanding of how the process of degradation occurs at the fine molecular level[2]. In this study, an analysis was carried out on how manufacturing of the chosen polymer blend [PLA-PBAT] is done using cotton-seed oil. Biopolymers are often manufactured from a combination of biological substances and in this research study, an attempt is made to provide an understanding of the chosen bio-polymer

*Author for correspondence

material with cotton-seed oil being the raw material used. In recent years, few studies have attempted to both classify and concurrently bring together various types of raw materials, which are of biological origins, such as (i) polysaccharides, and (ii) other plant-based raw materials, from which manufacture of several types of bio-polymers can be easily done using by-products of the crop produce.

In this research study, an attempt to establish degradation of the chosen biodegradable polymer blend [PLA-PBAT], with a 60:40 ratios, was the basis with the prime objective of establishing how the intricacies specific to the degradation process occurs when mixed with soil coupled with the occurrence of gradual decomposition, or degradation, of the chosen polymer blend [PLA-PBAT]. This phenomenon has been studied using a few techniques. One such technique is IR spectroscopy. This research paper attempts to provide an understanding of how the actual degradation occurs in real-time conditions[4,5]. This will help in both enabling and establishing an understanding of how the chosen polymer blend [PLA-PBAT] acts as a packaging substance while concurrently helping to understand the material that is being used to study degradation[6]. Degradation of the most widely chosen and used a variety of biopolymer blends, i.e., PLA-PBAT, is examined. This helps in establishing the time that is required for 100 per cent degradation of the chosen biopolymer material by the use of statistical modelling technique.

Montgomery and co-workers[7] contributed to providing an understanding of simple linear regression modelling, and how the modelling can be done manually using the desired equations. Their approach essentially makes use of statistical modelling, based on simple linear regression, as a viable alternative that is suitable for the purpose of both studying and establishing the degradation of the chosen biopolymer blend, i.e., PLA-PBAT.

2.0 Conditions for Environment-Induced Degradation of the Chosen Biopolymer

Degradation can be considered to be a desirable quality of any bio-degradable polymer and a proper statistical study of degradation of the chosen biopolymer of interest is limited in the published literature. Herein, the degradation is considered to be influenced by one major factor, which is time. The percentage degradation at a given specific time is a desirable result for any polymer blend. The degradation essentially varies with the type of environment, soil content, and a few other natural factors, which tend to exert an influence on the rate of degradation. In this study, the analysis conditions for the reaction mixture and percentage degradation of the chosen polymer blend samples are as follows:

2.1 Conditions for the Reaction Mixture

Origin of compost: Livestock excrement, municipal and vegetable waste.

Reaction temperature:	58°C (±2°C)
Dry solid (%):	61.2
Volatile content (%):	39.5

CO_2 evolved during first 10 days in blank vessel: 61.1mg/gm of volatile content of compost

Test duration:	117 days.
Reference material:	Cellulose
Volume of reaction vessel:	3000ml
pH for the test medium:	Before-7.6, After -7.3

2.2 Percentage Degradation Relative to the Chosen Reference Material [i.e., Cellulose]

Sample:	90.04%
Reference (Cellulose):	~100%

3.0 Simple Linear Regression

In this research study, the biodegradation (%) of the sample was considered to be dependent on time (days) where a single variable acts as a major factor in influencing the amount of the degradation. Regression modelling was used to determine the best fit for degradation of the chosen biopolymer sample. Since a single variable acts as the dependent, simple regression modelling was used for the purpose of performing regression analysis (Figure 1).

The simple linear regression analysis is a statistical modelling technique that enables in the study with variable 'X' being the independent variable and variable 'Y' being the dependent variable. The simple linear regression model is given by the equation $Y = \alpha + ßX$, which describes a line, with ß being the slope of the line and α being the Y- intercept.

Simple linear regression was used since thetwo key factors to consider are: (i) Biodegradation (%), and (ii)

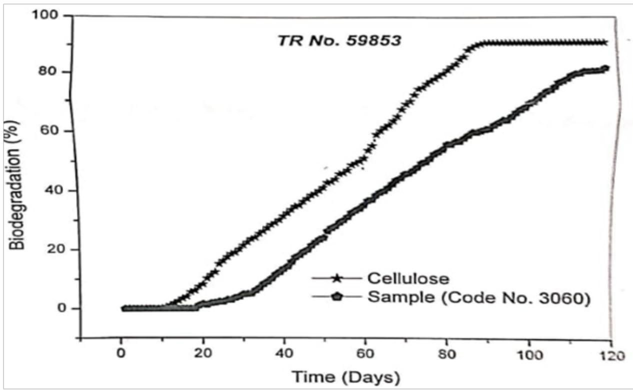

Figure 1. Variation of degradation (percent) of both the reference material, i.e., cellulose and the polymer sample [PLA-PBAT] with time (days). Plot based on data taken from the Interim report of Bio green biotech company.

Time (days). These two factors tend to act as deciding factors for the purpose of manufacture of the chosen polymer blend [i.e., PLA-PBAT].

4.0 Regression Modeling

Simple linear regression modelling was done using a statistics tool [IBM SPSS]. Here the data input was taken from the interim report of Bio Green Biotech, a biopolymer company. The data documented in Table 1 provides a compilation of the time (days) and biodegradation (%), which are the X coordinate and Y coordinate in the Cartesian form. This data is then recorded in excel (xls) format. From the excel data, the chosen software performs the modelling. The reference material for purpose of modelling is ignored, with the modelling being done on the chosen biopolymer (PLA-PBAT) sample.

Based on the available input data for the chosen biopolymer sample of interest the modelling, using simple linear regression, was done using IBM SPSS. The variation of degradation (per cent) with time (days) is shown in Figure 2. From the graph, it is observed that for the chosen biopolymer sample the variation of degradation (per cent) with time (days) is essentially linear and can safely be expressed using the relationship $Y = \alpha + ßx$. Regression modelling was then done on the graph, which depicts the variation of degradation (percent) with time (days). The resulting output is as follows:

The regression model reveals the R Square value to be 0.968, and the adjusted R Square value to be 0.965. In terms of percentage the regression fit for R Square = 96.8%, and the adjusted R Square value is 96.5% to account for a better fit for the chosen biopolymer sample [PLA-PBAT].

The ANOVA for degradability based on the sum of squares (SS_T) was 10564.308 with the standard error for time (days) being 0.041.

To provide a better fit for the variation of degradation (%) with time (days) and less chance for error the regression was done on the as-provided test data for a second iteration. Following the second iteration, the regression analysis reveals the slope of the curve or plot to increase and the degradation is close to 100% after 120 days. The regression modelling was done on data shown in Figure 3 and the resultant output is summarized in Figure 4.

The regression model for the second iteration reveals the R Square value to be 0.986, and the adjusted R Square value to be 0.984. In terms of percentage 002C the regression fit for R Square was 98.6% and the adjusted R Square value was 98.4%, thereby providing a better fit for the test data on the chosen biopolymer [PLA-PBAT] sample. The ANOVA for degradability for the sum of squares (SS_T) was 15415.077 with the standard error for time (days) being 0.033 (Figure 5).

5.0 Interpretations of Test Results

Based on the results obtained, the following inferences are drawn:

- After the 1st iteration the variation of degradation (percentage) with time (days) reveals the actual degradation percentage i.e., 90% and the time required for degradation is 120 days.
- The R-Square value for the first iteration is 96.8%, which suggests that the modelling is done.
- Up to a degradation percentage of 90%. Following the second iteration, the R-square value is adjusted to 96.5%.
- The R-Square value for the first iteration is 98.6%, which suggests that modelling is done up to a degradation percentage of 100%. After the second iteration is done, the R-Square value is adjusted to 98.4%, and the graph is extrapolated beyond 120 days.
- From the R-Square value we can safely use the model for other material blends having the varied proportion of biopolymers. This technique will help in obtaining

The data input for purpose of the analysis is:

Table 1. Data required for the purpose of statistical modelling

Time (days)	Biodegradation (%)
0	0
10	10
20	15
30	18
40	20
50	25
60	35
70	43
80	50
90	68
100	74
110	82
120	90

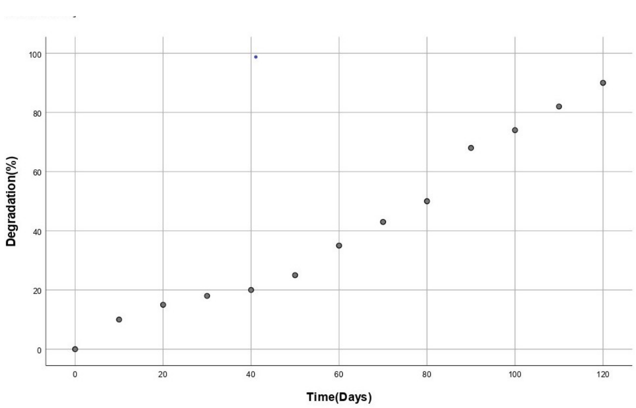

Figure 2. Variation of degradation (percent) with time (days) for the chosen biopolymer sample [PLA-PBAT].

the time (in days) that is required for complete degradation. In real-time situations, when the test for the degradation is done, the time that is taken is proportional to the actual time that is required for degradation of the chosen biopolymer material.

- Also, in the developed and proposed model the standard error for the estimate is reduced from 5.574 to 4.469 or a reduction of 1.105. Here the estimated error takes into consideration the whole model, which provides the overall data output for the simple linear regression model.

Regression

Variables Entered/Removed[a]

Model	Variables Entered	Variables Removed	Method
1	Time(Days)[b]	.	Enter

a. Dependent Variable: Degradation(%)
b. All requested variables entered.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.984[a]	.968	.965	5.574

a. Predictors: (Constant), Time(Days)

ANOVA[a]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	10222.505	1	10222.505	328.984	.000[b]
	Residual	341.802	11	31.073		
	Total	10564.308	12			

a. Dependent Variable: Degradation(%)
b. Predictors: (Constant), Time(Days)

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	-4.198	2.922		-1.437	.179
	Time(Days)	.749	.041	.984	18.138	.000

a. Dependent Variable: Degradation(%)

Figure 3. Result obtained after regression analysis.

Graph

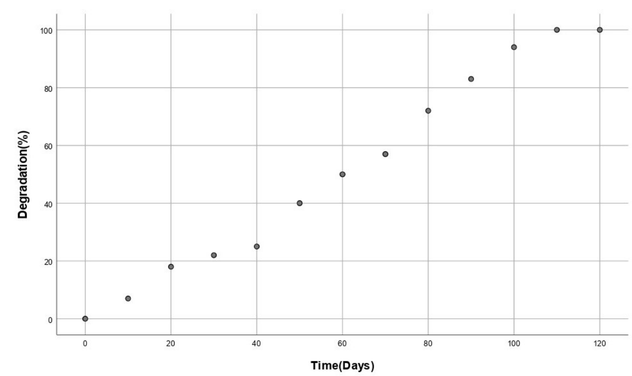

Figure 4. Variation of degradation with time following second iteration of the available data on the chosen biopolymer sample [PLA-PBAT].

- The error for time (days) during modelling is reduced from 0.041 to 0.033, with the difference of 0.08. This does influence the quality of the end result after the modelling is done. Thus, performing successive iterations tends to reduce the error while providing an end result with real time data, which helps in providing overall goodness of fit to the plot depicting the variation of degradation (percentage) with time (days). This is essential for an analysis of the data, which has a relatively low error value and thereby

Regression

Variables Entered/Removed[a]

Model	Variables Entered	Variables Removed	Method
1	Time(Days)[b]	.	Enter

a. Dependent Variable: Degradation(%)

b. All requested variables entered.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.993[a]	.986	.984	4.469

a. Predictors: (Constant), Time(Days)

ANOVA[a]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	15195.434	1	15195.434	761.007	.000[b]
	Residual	219.643	11	19.968		
	Total	15415.077	12			

a. Dependent Variable: Degradation(%)

b. Predictors: (Constant), Time(Days)

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	-3.440	2.342		-1.469	.170
	Time(Days)	.914	.033	.993	27.586	.000

a. Dependent Variable: Degradation(%)

Figure 5. Result obtained following Second iteration and regression analysis.

tends to directly affect, or influence, the modelling data.

- Here the F value in the ANOVA for the second (2nd) iteration is increased twice as that for the first (1st) iteration result. This reveals the trend for which the null hypothesis is rejected and the predictive power of the dependent variable, that is degradation (%), for the purpose of analysis of the data analysis using the model holds true.

6.0 Conclusions

In this short, novel and informative research study following are the key findings:

- A statistical modelling technique to explain the degradation of commonly chosen and used biopolymer blends [PLA-PBAT].
- Here the data for purpose of the analysis is obtained from real-time degradation up to 90%. This data is then fed into a statistical tool, i.e. IBM SPSS, and carefully analysed for two successive iterations.
- The data for variation of degradation (per cent) with time (days) is analysed. This data is an enhancement of the real-time data, which helps in determining the goodness of fit for which the model holds good, or is applicable, for the relevant and applicable data.
- An increase in the 'R' Square value and an increase in the 'F' value of the chosen model reveals the data input and data fit to be good. This suggests that statistical analysis can be used for both the prediction and analysis of the test data specific to the degradation of the chosen biopolymer material.
- Use of statistical modelling for the study of degradation of biopolymeric materials will be helpful in putting to effective use the real-time data while the chosen statistical modelling technique will be helpful in reducing the time that is required for the purpose of analysis of the degradation of the chosen biopolymer.
- Given the paucity of information in the field of analysis specific to biopolymers, i.e., degradation and its overall influence on the environment, additional studies are needed prior to ensuring the successful implementation of biopolymers as a viable and attractive alternative to plastics for use in a spectrum of applications relevant to daily life.

7.0 Acknowledgements

The input data used in this study was taken from an Interim report of the company BIOGREEN Biotech (Bangalore, India). This data was used as the basis for the purpose of statistical modelling that is presented in this paper.

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