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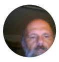

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Mathematical Modeling of the Biodegradation Process of Biodegradable Material and Performance Comparison

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Abstract: **-**The paper presents a mathematical model of the biodegradation process of plastics. The main results of the mathematical model are three parameters which are measures of the biodegradation process. Biodegradation parameters are used to compare the biodegradation performance of materials, the prediction in time of the biodegradation process and, in future, to optimize the location of biodegradation.

Key-words: biodegradation, measures, mathematical, model, biodegradable, plastic

1 Introduction

Our attempt started from the need to compare biodegradable plastic products based on starch [3] and [5], with other biodegradable products. For this comparison it should be found a parameter (a measure) that is widely accepted as a measure of the biodegradation process. Time variation curve of the carbon dioxide concentration, emitted in the biodegradation process, being the most common characteristic of this process, was chosen in order to obtain such a parameter. From this curve was obtained the curve of biodegradation degree, more general notion, which means the amount of carbon emitted by biodegradation in relation to the amount of carbon contained in material, after [5]. In the proposed mathematical model we have identified three process parameters, possible measures of the biodegradation process: the decomposition limit of the material, the rate of decomposition and the damping characteristic.

2 Problem Formulation

Mathematical modeling of the biodegradation process using experimental curve of evolution of carbon dioxide released is done to determine the characteristic parameters (measures) of the process. Finally these parameters will be used to compare the performance of biodegradation of materials. Also, these parameters highlights the inherent characteristics of the material and the conditions for conducting the process of biodegradation, too. For clarity resume some remarks from [2]. As defined method for measuring biodegradation, after [3] or [6], measuring the degradation process can be done several ways. Micro-aerobic activity can be measured by the amount of oxygen consumed or the amount of carbon dioxide produced from the degradation phenomenon. The quantity of methane or gas mixture produced in the anaerobic degradation by microbes is also a measure of the degradation process. In [6] appears similar graphics parameters biodegradability. In [4] are given the same definitions for the measures of the degradation capacity of a material, but there are important details on the duration of complete degradation for cotton, paper, orange or banana peels, nylon etc. This last measure is a good measure of biodegradation capacity of materials and can be useful for predicting the accumulation of waste. Obviously, there are possible other characterizations of biodegradability of a product (maximum limit of biodegradability, speed of biodegradation, the amount of waste resulting from biodegradation etc.).

3 Problem results

To characterize the biodegradation capacity of a material takes over the method of [5], [3] and [4], which uses variation in time of the concentration of carbon dioxide resulting from decomposition. Mode and materials are described in [5]. Our problem is the interpolation of experimental data of carbon dioxide releases given in [5], with a function that contains parameters that have physical significance for the biodegradation process. To give a degree of universality to the biodegradation measures, they will be expressed in degree of biodegradability which means the ratio of actual amount of carbon through decomposition and the resulting total amount of carbon contained in the material, after [5].

Experimental data from starts are summarized in Fig. 1. Reading points with coordinates: the number of days from starting the process, namely carbon dioxide concentration (converted to the degradation degree), are graphically in Figure 1, which appears linear interpolation of these data, too.

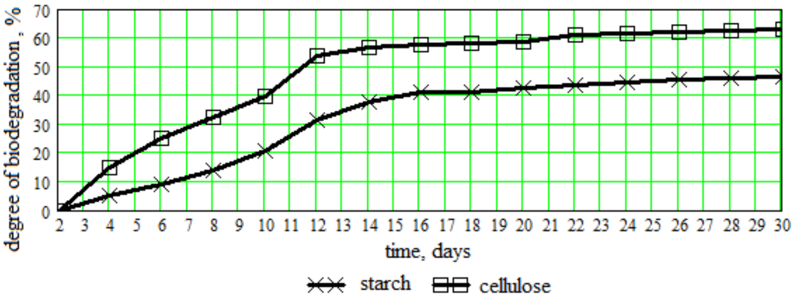

Fig. 1 Experimental data taken from [1]. Are marked the days on which readings were made, the reading points being joined by linear interpolation

It is noted that the biodegradation evolution curve seems to have finally an almost horizontal ceiling. Mathematically speaking, this behavior suggests the existence of a horizontal asymptote of the degree of biodegradation. However, this suggestion is not mandatory, but we cannot allow an infinite increase of the concentrations. In addition, the function must be increasing over the whole domain of definition: from zero to plus infinity. To model this behavior we have proposed a curve of the form:

$$C(t) = a - b \cdot e^{-\alpha \cdot t}. \qquad (1)$$

In formula (1), C represents the degree of biodegradability as subunit number, t is time in days, and a, b and α are parameters whose meaning will be discussed further, e = 2.71 ... is the natural logarithm base. To express the degree of biodegradation in percentages, the function C is multiplied by 100, which is still valid. The values of these parameters can be found by the method of least squares, minimizing the functional:

$$F(a,b,\alpha) = \sum_{i=1}^{n} \left(a - b \cdot e^{-\alpha \cdot t_i} - C_i \right)^2. \qquad (2)$$

In formula (2), t_i and C_i are the coordinates of the experimental data, in number of n pairs. Minimize functionality (2) can be numerically and, for the three parameters are the values: in the case of starch, a = 0.539, b = 0.685, α = 0.085 per day, and for cellulose: a = 0.653, b = 0.882, respectively α = 0.139 per day. The best approximation of type (1) for the degradation curve of starch based packaging which is shown in the Figure 1 is the function:

$$C(t) = 0.539 - 0.685 \cdot e^{-0.085 \cdot t}, \qquad (3)$$

and for cellulose:

$$C(t) = 0.653 - 0.882 \cdot e^{-0.139 \cdot t}. \qquad (4)$$

In the Figure 2 are given together the experimental points and the curves obtained by interpolating them. Curves, which have horizontal asymptote $C = a = 0.539$ (53.9% biodegradation) for starch based packaging, and $C = a = 0.653$ (65.3% biodegradation) for cellulose, allow the extrapolation of results, too. Thus, the limit values would be, according the model (1), the maximum amount of carbon dioxide ceded by the materials trough biodegradation.

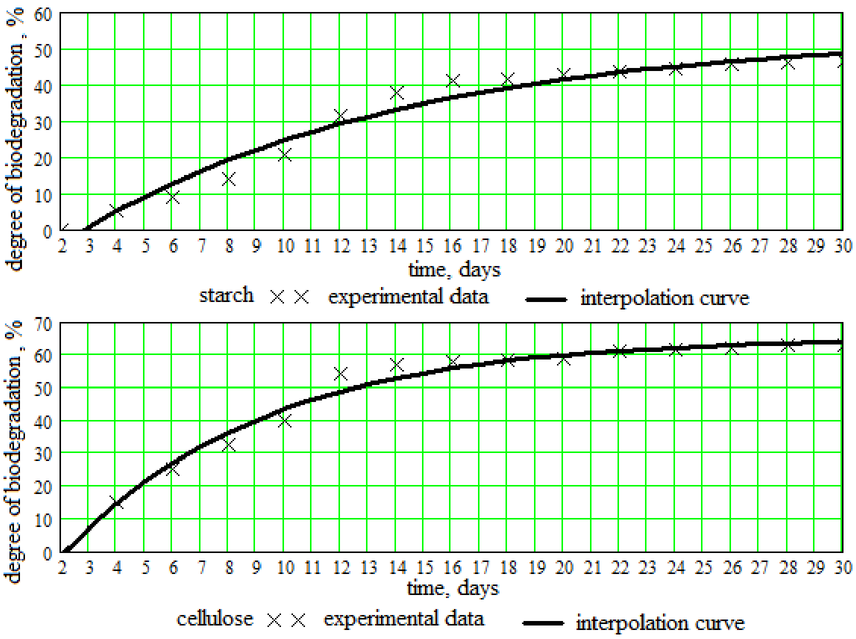

Fig. 2 Interpolation curve (3) and experimental points on the same graph.

By derivation of (1) with respect to the time *t*, we obtain a function that describes the temporal variation in growth rate of the concentration of carbon dioxide:

$$\frac{dC}{dt} = \alpha b \cdot e^{-\alpha t}. \tag{5}$$

If we note the initial rate of biodegradation:

$$w = \alpha b, \tag{6}$$

then, the formula (1) can be put in the form:

$$C(t) = a - \frac{w}{\alpha} \cdot e^{-\alpha \cdot t}. \tag{7}$$

There was thus the initial rate of biodegradation parameter, *w*. Finally, the parameter α can be interpreted as a damping factor, due to the size, even as a damping frequency of biodegradation process. Graphical representation of biodegradation rate variation is shown in the Figure 3 (extrapolated version) and noticed that from day 45 the biodegradation rate nearly canceled.

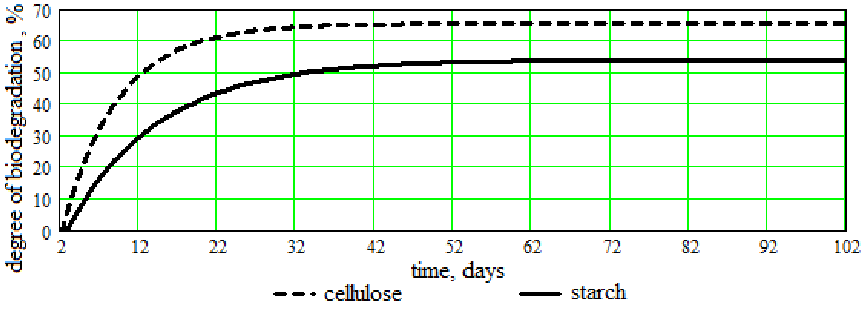

Fig. 3 Extrapolation of the results obtained by interpolating experimental data with an interval of 102 days.

On the representation (7) of the variation in time of the biodegradation degree of a material, the main qualitative parameters such as: limit the degree of biodegradation decomposition, *a*, the biodegradation rate, *w*, the damping factor of the degradation process, *α*.

3.1 Discussion

The phenomenon of materials biodegradation and performance of this process depends on external factors: temperature, humidity, concentration of specific substances in the atmosphere of the area in which the material undergoes this process, radiation, etc. Theoretical considerations can be developed taking into account these factors and performing experiments and processing complex.

Noting with T temperature, u humidity, p atmospheric pressure, with c_i initial concentration of carbon dioxide in the medium, r the amount of ultraviolet radiation, can complicate the formula (7), making the parameters a, b and α to depend on temperature, humidity, pressure, initial concentration of carbon dioxide and the amount of ultraviolet radiation

$$C(t) = a\left(T,u,p,c_i,r\right) - \\ -\frac{w\left(T,u,p,c_i,r\right)}{\alpha\left(T,u,p,c_i,r\right)} \cdot e^{-\alpha\left(T,u,p,c_i,r\right)\cdot t} \cdot \tag{8}$$

It may take into account that, in turn, these parameters are dependent on time, so you can get a more accurate temporal prediction of performance biodegradation process. A first approximation of the dependence of the four parameters introduced can be formulated as follows:

$$a(T,u,p,c_0,r) = a_0 \cdot f_{Ta}\left(\frac{T}{T_0}\right) \cdot f_{ua}\left(\frac{u}{u_0}\right) \cdot \\ \cdot f_{pa}\left(\frac{p}{p_0}\right) \cdot f_{ca}\left(\frac{c_i}{c_{i0}}\right) \cdot f_{ra}\left(\frac{r}{r_0}\right) \quad , \tag{9}$$

$$w(T,u,p,c_0,r) = w_0 \cdot f_{Tw}\left(\frac{T}{T_0}\right) \cdot f_{uw}\left(\frac{u}{u_0}\right) \cdot \\ \cdot f_{pw}\left(\frac{p}{p_0}\right) \cdot f_{cw}\left(\frac{c_i}{c_{i0}}\right) \cdot f_{rw}\left(\frac{r}{r_0}\right) \quad , \tag{10}$$

$$\alpha(T,u,p,c_0,r) = \alpha_0 \cdot f_{T\alpha}\left(\frac{T}{T_0}\right) \cdot f_{u\alpha}\left(\frac{u}{u_0}\right) \cdot \\ \cdot f_{p\alpha}\left(\frac{p}{p_0}\right) \cdot f_{c\alpha}\left(\frac{c_i}{c_{i0}}\right) \cdot f_{r\alpha}\left(\frac{r}{r_0}\right) \quad , \tag{11}$$

where the parameters T, u, p, c_i, r with zero representing normal atmospheric conditions, so conventional values, and the functions f indices concerned are functions that depend on ratios of current values of the parameters and conventional values. The parameters a_0, w_0, α_0 and r_0 are calibration constants. Forms of functional dependencies (9), (10) and (11) will be determined experimentally as calibration parameters.

4 Conclusions

Comparison of two biodegradable materials can be done on the base of the results presented in this article. Note that the cellulose is degraded in higher proportion than the starch-based packaging. On the other hand, in the Figure 4 follows that the degradation rate of cellulose is higher than the starch packaging within first 12 days, then becomes smaller until, at about 50 days, after which the differences are negligible. All these observations are valid in atmospheric conditions in which degradation tests were conducted.

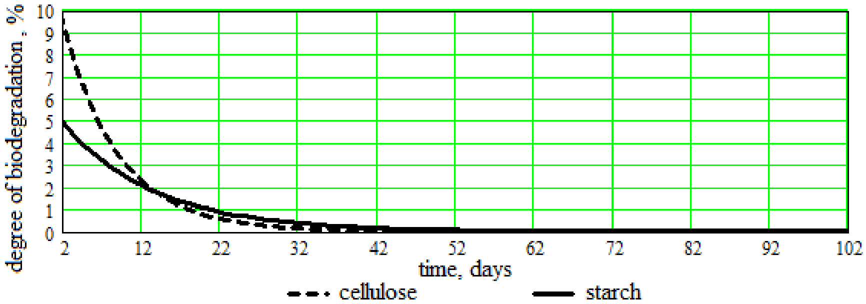

Fig. 4 Variation in time of the biodegradation rate for the starch and cellulose packaging

The results provided in this article shall apply primarily to: comparing biodegradation capacity of materials, optimization or improvement schemes for the degradation of biodegradable materials and obtain data that can be used in a more complex mathematical model of the biodegradation process.

References:

[1] Cioica Nicolae, Coţa Constantin, Nagy Mihaela, “The influence of glycerol contents on the expansion index of starch based loose fill packaging obtained through thermoplastic extrusion” INMATEH 2009-III, Bucharest, nr. 29, pag.52-58.

[2] Cârdei Petru, Paul Maria, Cioica Nicolae, Naghy Emilia Mihaela, Mathematical model for assessing characteristics of packages biodegradation starch-based shock absorbent packaging, INMATEH – *Agricultural Engineering*, VOL. 32, no. 3/2010, pp. 93-99.

[3] http://en.wikipedia.org/wiki/Biodegradation.

[4] http://www.associatepublisher.com/e/b/bi/bio.

[5] Paul Maria, Cadar Oana, Cadar Sergiu, Levei Erika, Pojar-Fenesan Maria, Balea Ana, Biodegradability Determination of Vegetal Originated Packaging Materials under Controlled Composting Conditions, *Agriculture - science and practice*, Nr. 1-2(73-74)/2010, pp. 77-83.

[6] Sadeghi M., Mesdaghinia A., Badkoubi A., Nabizadeh R. and Khavanin A., Application of the Ozonation Pre-treatment for Biodegradation of Aqueous Solutions of Methyltert-Butyl Ether, *American Journal of Environmental Sciences* 1 (1): ISSN 1553-345 X © Science Publications, 2005, pp. 41-45.