Contemporary Engineering Sciences, Vol. 11, 2018, no. 12, 559 - 570
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/ces.2018.8251

Predicting Mechanical Properties of Thermoplastic Starch Films with Artificial Intelligence Techniques

Cesar Guzman

Escuela de Ciencias Básicas Tecnología e Ingeniería
Universidad Nacional Abierta y a Distancia, Sede Nacional JCM
Calle 14 Sur No. 14 – 23
Bogotá D.C., Colombia

Sofía Collazo-Bigliardi

Instituto de Ingeniería de Alimentos para el Desarrollo
Universidad Politécnica de Valencia, Camino de Vera s/n
46022 Valencia, Spain.

Rodrigo Ortega-Toro

Facultad de Ingeniería, Dpto. de Ciencias de los Alimentos, Grupo IFCRA
Universidad de Cartagena, Cra. 6 #36-100
Cartagena de Indias D.T. y C. Colombia

Abstract

Biodegradable polymers have similar physicochemical properties than conventional polymers, but they can be degradable under controlled conditions in less than 180 days. Thermoplastic starch films have a relative importance because of their low cost, high production and good processability by conventional techniques like melt blending, compression molding, extrusion, among others. However, they present several drawbacks (poor mechanical properties, high water vapor permeability, and retrogradation) that limit their industrial applications. In the present paper, we developed a computer tool, which employs artificial intelligence techniques to predict the values of the physical properties of thermoplastic starch materials without having to resort to the elaboration of the physical parts. Our tool allows the industry to reduce time, resources and costs.

Keywords: thermoplastic starch, artificial intelligence, mechanical properties

1 Introduction

The industry of conventional polymers has been constantly grown since 1950 with the development of petrochemistry. In 2014, global production of conventional polymers was 300 millions tons Shen et al. [10]. The expansion of polymer industry has generated several contaminants on resources of soil and water causing a high concern in academia and industry. For this reason, development of biodegradable polymers Avérous and Pollet [2] is a suitable option. Biodegradable polymers have similar physicochemical properties than conventional polymers, but the first one can be degradable under controlled conditions in less than 180 days. Natural polymers as carbohydrates and proteins are frequently used for developing these materials. Among them, starch has a relative importance because of their low cost, high production and good processability by conventional techniques like melt blending, compression molding, extrusion, among others Ortega-Toro et al. [7]. However, this kind of materials presents several drawbacks (poor mechanical properties, high water vapor permeability, and retrogradation) that limit their industrial applications.

Artificial Intelligence techniques are helping industries to improve their efficiency and performance in a great variety of applications: education Rani et al. [8], space Tonutti et al. [11], He et al. [6], space exploration Guzman et al. [5], manufacturing Wilson [12], Rao et al. [9], etc. The development of a computer program, that employs artificial intelligence techniques to predict the values of the physical properties of the materials mentioned above without having to resort to the elaboration of the physical parts of biodegradable thermoplastic starch, will be a great utility to extend its industrial application: allowing to reduce time, resources and costs.

This paper is organized as follows. Section 2 outlines the materials and the current process to calculate the values of the physical properties. Section 3 presents our novel predicting solution that estimates the values of some physical properties of biodegradable thermoplastic starch using a predictive model which is explained in Section 4. Section 5 describes some evaluations and discussions of our approach, and, finally, the last section concludes and outlines future research lines.

2 Materials and current method calculation

In this section, we explain the current overall process to elaborate biodegradable thermoplastic starch films (flexible materials). We describe the materials that we used, along with the physical properties that we chose to study.

The more important physical properties are the **tensile properties**, which indicate how the material will react to forces applied in tension. These properties are important because they give information about the behavior of the film under different forces or conditions. Industry uses the tensile properties to design materials for specific applications such as bags, trays, and boxes.

Tensile properties refer to the final use of the material. For example, a packaging material should have physical properties suitable for containing a product without any visible damages. We study the following tensile properties of thermoplastic starch films:

- Tensile strength ($\mathcal{TS}$). It provides information about the maximum stress that a material can withstand under tension before its cross-section significantly shrinks, and break. $\mathcal{TS}$ is a relevant property because it gives information about the final use of the material. For example, the weight of foods that a bag could contain without the material break.

- Elastic modulus ($\mathcal{M}$). It is a number that measures a film's resistance to being deformed elastically when a force is applied to the film. The $\mathcal{M}$ of an object is defined as the slope of its stress–strain curve in the elastic deformation region. This parameter is a measure of the rigidity of the material. This means how many force can be applied to the material before this one suffers a permanent deformation. When a force is applied to a flexible film, the material is deformed in two steps. The first step is a non-permanent deformation or elastic deformation (if the force disappears, the material can recover their original shape). The second step is a permanent deformation or plastic deformation (if the force disappears, the material can not recover their original shape). In this way, the elastic modulus is a measure of the resistance of the material to elastic deformation.

- Elongation ($\mathcal{E}$) of the films. It is the deformation of the material when a longitudinal force acts on it. As was mentioned before, when a force is applied to a flexible material, this material suffers an elastic deformation followed by a plastic deformation. Just at the final of the plastic deformation, the film is broken. The last value of deformation registered before the breaking is the parameter $\mathcal{E}$ expressed in terms of percentage.

We elaborated the films of starch obtaining the corn starch from Almidones de Sucre S.A.S. (Sincelejo-Corozal, Sucre, Colombia). Its moisture content was

9% (w/w) and amylose percentage was 15%. We purchased the glycerol from Panreac Química, S.A. (Castellar del Valles, Barcelona, Spain).

2.1 Preparing the Films

Native starch and glycerol, as plasticizer, were dispersed in water. The starch:glycerol ratio was 1:0.3. The formulations were hot-mixed on a two-roll mill at 130 ºC and 10 rpm for 20 min. A trowel was used during mixing to smoothly spread the material on the rolls. The paste sheet formed was removed from the mill and conditioned at 25 ºC and 53% relative humidity (RH), using a $Mg(NO^3)^2$ saturated solutions for 72 h.

Afterwards, films were obtained by compression molding. Four grams of the preconditioned paste were put onto steel sheets and pre-heated on the heating unit for about 5 min. Compression molding was performed at 150 ºC for 2 min at a pressure of 30 bars, followed by 6 min at 130 bars; thereafter, the cooling cycle was applied for 3 min. The films were conditioned at 25 ºC and 53% RH for 1 week for mechanical characterization.

2.2 Characterizing the film: thickness and tensile properties

We used a Palmer digital micrometer to measure film thickness to the nearest 0.0025 mm at six random positions around the film. A universal test machine was used to determine $\mathcal{TS}$, $\mathcal{M}$ and $\mathcal{E}$ at break point of the films, following ASTM standard method D882 ASTM [1]. Dimensions of samples were 2.5 cm wide and 5 cm long. Equilibrated samples were mounted in the film-extension grips of the testing machine and stretched at 50 mm min - 1 until breaking. $\mathcal{M}$, $\mathcal{TS}$, and $\mathcal{E}$ were determined from the stress–strain curves, estimated from force–distance data obtained for the different films. At least ten replicates were obtained from each sample.

3 Predicting the mechanical properties

In this section, we explain the overall process to predict the values of the three mechanical properties $\mathcal{TS}$, $\mathcal{E}$, and $\mathcal{M}$. Our work combines two techniques of the artificial intelligence, the Monte Carlo Simulation and the prediction of values through the machine learning.

We performed a Monte Carlo Simulation in order to estimate the values of the mechanical properties. The aim of the Monte Carlo is to simulate the real process explained in Section 2 in order to calculate $\mathcal{TS}$, $\mathcal{E}$ and $\mathcal{M}$. More specifically, during the simulation we estimate the values of $\mathcal{TS}$ with a predictive model and basing on the value of $\mathcal{TS}$ we estimate the value of $\mathcal{E}$. Once we choose the values of $\mathcal{TS}$ and $\mathcal{E}$, we calculate the property $\mathcal{M}$ as the average of the first ten slopes that are calculated during the simulation as the ratio of two distinct points formed by values of $\mathcal{TS}$ and $\mathcal{E}$. This will be explained in more detail in Section 4.

From the real process, we detected some input parameters that we used to estimate the values of the mechanical properties:

- X_1 = Pressure exerted. It is the force that we applied to the material. We applied a exerted pressure of 0,8333
- X_2 = Starch. We used a 71,3% of starch.
- X_3 = Glycerol. We used a 21,4% of Glycerol.
- X_4 = Water. We used a 7,3% of Water.
- X_5 = Thickness. The material has a thickness of 0,391 mm
- X_6 = Width. The material has a width of 0,025
- X_7 = Length. The material has a length of 0,05
- X_8 = Time. It represents a given time instant in which we calculate the estimated value of $\mathcal{TS}$, and $\mathcal{E}$. The time starts in 0 and ends in a fixed value timeMax := 40 sec, which is the average duration of the real process. The values of $\mathcal{TS}$ and $\mathcal{E}$ are measured each 0.04 sec, that is, the time is increased by 0.04 sec.

Such as we will explain in Section 4, we use the parameters $\{X_1, \ldots, X_8\}$ as the input data for the predictive model which estimates the value of $\mathcal{TS}$ at a given time instant. We namely those parameters as **input parameters for the model**.

Algorithm 1 describes the process to estimate the values of the mechanical properties. The first part of the algorithm (lines 1 - 5) initializes the variables and load a predictive model that will be used to estimate the value $\mathcal{TS}$ at a given time. We will explain our predictive model in the next Section. Next, the algorithm performs a Monte Carlo Simulation (lines 6 - 13) in order to determine the precise moment of time where the material can be broken because of the exerted force. We said the material is broken due to the exerted force when the slope is less or equals to zero. For instance, Figure 1 shows the plot of the exerted force against the elongation of the material, resulting in the line blue. We can see that the material is broken (red circle) when the applied tensile strength is more or less 7,45. That is, at that moment the slope is equal or less than zero.

Require: EstimateValues(timeMax:=40,increase:=0.04,fixedValue:=5,parametersModel)
1: slopeTemp := ∞
2: model := load the predictive model
3: $\mathcal{TS}$' := {}
4: $\mathcal{E}$' := {}
5: slope' := {}
6: **for** time = 0 **to** timeMax **and** slopeTemp > 0 **do**
7: $\quad$ $\mathcal{TS}'_{time} \leftarrow$ **predictValue**(model, parametersModel,time)
8: $\quad$ distance $\leftarrow$ time * forceExerted
9: $\quad$ $\mathcal{E}'_{time} \leftarrow \ln(\frac{length-(1-\frac{distance}{1000})}{length})$
10: $\quad$ **if** size($\mathcal{TS}$') > fixedValue **then**
11: $\qquad$ old := time - (fixedValue*increase)
12: $\qquad$ slopeTemp := **calculateSlope**($\mathcal{TS}'_{time}$,$\mathcal{TS}'_{time}$,$\mathcal{E}'_{time}$,$\mathcal{E}'_{old}$)
13: $\qquad$ slope'$_{time} \leftarrow$ slopeTemp
14: previous := time-increase
15: $\mathcal{TS} \leftarrow \mathcal{TS}'_{previous}$
16: $\mathcal{E} \leftarrow \mathcal{E}'_{previous}$
17: $\mathcal{M} \leftarrow$ average of first ten slope in slope'

Algorithm 1: Estimate the mechanical properties using predictive model.

Thereby, the simulation goes on while the condition slopeTemp > 0 holds and the time is less or equals than a fixed maximum time (variable timeMax), which is an average duration calculated from the real process (line 6). During the simulation, the algorithm calculates at each time the value of $\mathcal{TS}$ with the predictive model (line 7), the value of $\mathcal{E}$ (lines 8 and 9), and the slope (lines 12 and 13). The slope is calculated by finding the ratio of two distinct points (x, y) that form a line, where we consider x=$\mathcal{TS}$ and y=$\mathcal{E}$. For us, the two points at a given time are formed by ($\mathcal{TS}_{time}$, $\mathcal{E}_{time}$) and ($\mathcal{TS}_{old}$, $\mathcal{E}_{old}$), where *old* is an old time that can be fixed by the input parameter fixedValue:=5 (line 11).

We choose as valid the values $\mathcal{TS}$ and $\mathcal{E}$ of the previous time when the material is broken. The value of $\mathcal{M}$ is the average of the first ten calculated slope (line 17).

Discussions Also it is not in the scope of this paper, our algorithm can be improved to a computational time of O(log(time)) by using a binary search instead of a linear simulation. The binary search will look from a time bewteen 0 and 40 until the slope$_{time}$ is closest or equal to zero.

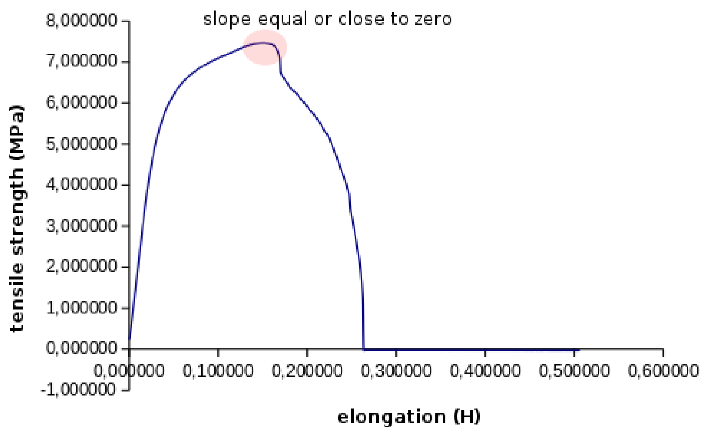

Figure 1: Material broken when the slope is less or equals to zero.

4 Predictive model

In this section, we explain the predictive model. We use the bagging predictive model Breiman [3], Xiao et al. [13] to estimate the value of $\mathcal{TS}$ at any given time.

Bootstrap aggregating or Bagging is an ensemble method that employs supervised machine learning methods for classification and regression Breiman [3]. Bagging trains multiple regression predictors in the ensemble using a randomly drawn subset of the training set. The predictors are combined by averaging the results of predicting a numerical outcome generating an aggregated prediction of multiple models which is less noisy than one calculated by an individual model.

Although there are several predictive models (boosting, stacking, random forest and others), we decided to use the bagging model because as a tree ensemble model it offers better predictions and it is a more stable model than other regression models Freund et al. [4]. Moreover, we emphasize the following reasons:

1. **approximate to nonlinear function problems**: bagging works well with problems that are linearly and non-linearly separable. In general, this is an advantage for tree ensemble models.

2. **performs well with large datasets**: it allows analysing significant amounts of data using standard computing resources in reasonable time.

3. **over fitting**: bagging takes care of overfitting in contrast to other ensemble models like Boosting that even though shows better predictive accuracy than bagging, it tends to overfit the training data as well.

In order to use the predictive model, we perform the following two steps: we first learning the model. Once the model is trained, we employed the model to estimate the value of the $\mathcal{TS}$.

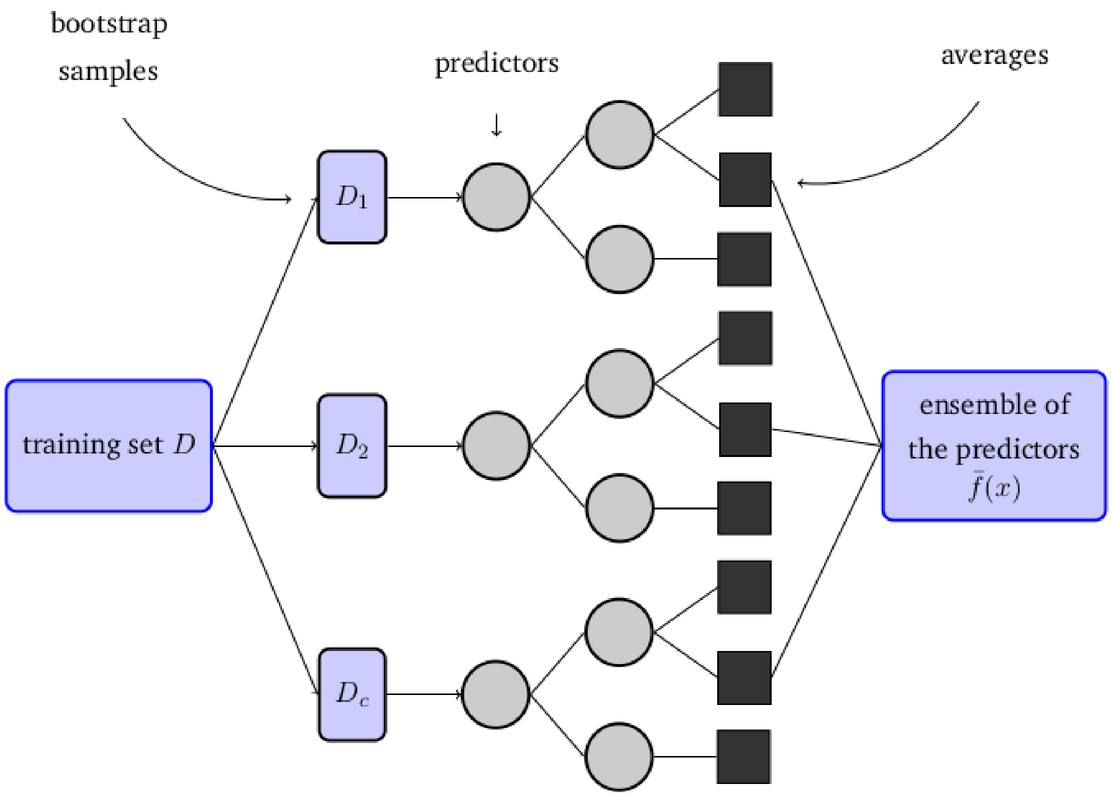

Figure 2: Operation of the bagging model, using model tress as base models.

To understand the bagging model, let us consider first the regression problem. Suppose we fit a model to the training sample set D={d_1,d_2,...,d_n}, obtaining the prediction $\bar{f}(x)$ at any given testing input x. As shown in Figure 2, bagging obtains the prediction as the average of the predictions of a collection of predictors with bootstrap samples [1], thereby reducing the variance of the prediction. For each bootstrap sample (new training sets) D_c / c={1,2,...,c}, bagging fits a predictor $\hat{f}_c(x)$. Then, bagging estimates the final prediction as a uniformly weighted average defined by:

$$\bar{f}(x) = \frac{1}{C} * \sum_{c=1}^{C} \hat{f}_c(x) \qquad (1)$$

[1]The basic idea of bootstrap sample is to randomly draw datasets with replacement from the training data

More specifically, bagging manipulates the training dataset to generate multiple explanatory parameters by sampling with replacement. In contrast to linear regression models, bagging can estimate variables with a long range of values, like the tensile strength $\mathcal{TS}$. The bagging model is trained with a benchmark that contains a set of real values of the input parameters for the model.

5 Results and Discussion

Our interest lies in to analyze the error of our estimating approach which employs a tree regression model that, in principle, can approximate nonlinear functions. We compare the predicted values of the three mechanical properties against the real values.

We obtained a set of real values of 6 different films (A, B, C, D, E, and F), each one with a benchmark of 995 data samples for a total benchmark of 5970 samples. We trained our predictive model with the total of the 5970 data samples, and we used this trained model in our process to predict the values of the mechanical properties.

We implemented the process in Java and all the experiments were run on a GNU/Linux Debian computer with an Intel ® Core (TM)2 Duo CPU P9400 @ 2.40 GHz, and 3GB RAM.

Table 1: Prediting the values of the mechanical properties of thermoplastic starch films.

film	**thickness** (mm)		**time** (sec)	$\mathcal{TS}$	$\mathcal{E}$	$\mathcal{M}$
A	0,391	real	9,84	7,465	15,133	183
		estimated	11,96	11,097	18,7	183,2
B	0,407	real	22,28	10,961	31,478	270,72
		estimated	22.48	10,963	31.82	275,81
C	0,368	real	23,8	11,88	33,304	345,82
		estimated	23,72	11,884	33,31	346,91
D	0,347	real	22,5	12,306	31,77	356,45
		estimated	22,68	12,302	32,063	362,62
E	0,384	real	25,6	10,667	35,424	275,38
		estimated	25,62	10,666	35,674	276,21
F	0,392	real	30,24	11,379	40,69	225,99
		estimated	31,06	11,429	42,182	226,43

Table 1 describes the results of applying our process to predict the values of the mechanical properties of six films with different thickness. For each film, we show two rows, one showing the real values and the second one showing the estimated values. The column Thickness is the only feature of the input parameters for the model that we changed in each film. Table 1 also shows the time of CPU (column **time**) to calculate the values of the mechanical properties, and the values of the mechanical properties. As we can see, our approach presents very closed results. The $\mathcal{TS}$ and the $\mathcal{E}$ in the film A was so much overestimated. However, the values of the same two properties in the other films were closer to the real time. One characteristic that we can remark is that our predictive model is overestimating, in more of the cases, the real values of the mechanical properties.

Table 2 summarizes the results of estimate the mechanical properties of the six films. The time of CPU is almost the same as to the time of the real process. As we mentioned in Section 3, this time can be improved in our algorithm. However, this is not in the scope of this paper.

Table 2: Summary of the values of the mechanical properties.

film		**time** (sec)	$\mathcal{TS}$	$\mathcal{E}$	$\mathcal{M}$
average	real	22,38	10,78	31,30	276,23
	estimated	23,01	11,39	32,39	278,53
σ^2	real	6,80	1,73	8,61	67,12
	estimated	11,27	0,61	15,29	68,65

In general, as it is shown in Table 2, the values of the mechanical properties were well estimated. This is a prove that the bagging model (which mean absolute error is $0,00379$ and the standard absolute error is $0,01067$) and, moreover, our approach work well to predict the values of the mechanical properties.

6 Conclusions

We have presented a novel method to estimate the values of the physical properties of thermoplastic starch films using artificial intelligent techniques. We demonstrated that we can use the state of the art of the Computer Science to solve problems of other branches of knowledge, such as the materials engineering.

We evaluated the performance of our novel method by conducting some experiments that estimate the values of the physical properties of several films. The purpose of the experiment was to check the available time and to evaluate the performance of our method. As far as we concern there is no other approach that solves the kind of problem that we presented in this paper. For this reason, we only compared our results with the values getting in the real process. All in all, the results support the conclusion: the accuracy of the model to estimate the values of the mechanical properties in time.

Finally, the results obtained for starch-based films indicate an excellent opportunity for future works in the prediction of the physicochemical properties of polymer matrices with higher complexity. This fact would reduce the cost and time that academy or industry need to obtain a formulation with the ideal properties for their products.

Acknowledgements. This work has been partly supported by the institution UNAD under the group Byte in Design.

References

[1] Designation ASTM. 882-88, Standard test Methods for Tensile Properties of thin Plastic Sheeting, Annual book of ASTM Standards, 8, 1989.

[2] Luc Avérous and Eric Pollet, Biodegradable polymers, Chapter in *Environmental Silicate Nano-Biocomposites*, Springer, 2012, 13-39. https://doi.org/10.1007/978-1-4471-4108-2_2

[3] Leo Breiman, Bagging predictors, *Machine Learning*, **24** (1996), no. 2, 123-140. https://doi.org/10.1007/bf00058655

[4] Yoav Freund, Robert E. Schapire, Experiments with a new boosting algorithm, *Machine Learning: Proceedings of the Thirteenth International Conference*, Vol. 96, (1996), 148-156.

[5] Cesar Guzman, Pablo Castejon, Eva Onaindia and Jeremy Frank, Reactive execution for solving plan failures in planning control applications, *Integrated Computer-Aided Engineering*, **22** (2015), no. 4, 343-360. https://doi.org/10.3233/ica-150493

[6] Yan-Lin He, Zhi-Qiang Geng and Qun-Xiong Zhu, A data-attribute-space-oriented double parallel (dasodp) structure for enhancing extreme learning machine: Applications to regression datasets, *Engineering Applications of Artificial Intelligence*, **41** (2015), 65-74. https://doi.org/10.1016/j.engappai.2015.02.001

[7] Rodrigo Ortega-Toro, Gabriella Santagata, Giovanna Gomez d'Ayala, Pierfrancesco Cerruti, Pau Talens Oliag, M Amparo Chiralt Boix and Mario Malinconico, Enhancement of interfacial adhesion between starch and grafted poly (e-caprolactone), *Carbohydrate Polymers*, **147** (2016), 16-27. https://doi.org/10.1016/j.carbpol.2016.03.070

[8] Monika Rani, Amit Kumar Dhar and OP Vyas, Semi-automatic terminology ontology learning based on topic modeling, *Engineering Applications of Artificial Intelligence*, **63** (2017), 108-125.
https://doi.org/10.1016/j.engappai.2017.05.006

[9] R. Venkata Rao, Dhiraj P. Rai and Joze Balic, A multi-objective algorithm for optimization of modern machining processes, *Engineering Applications of Artificial Intelligence*, **61** (2017), 103-125.
https://doi.org/10.1016/j.engappai.2017.03.001

[10] Li Shen, Juliane Haufe and Martin K Patel, *Product Overview and Market Projection of Emerging Bio-based Plastics Pro-Bip 2009*, Report for European polysaccharide network of excellence (EPNOE) and European bioplastics, 243, 2009.

[11] Michele Tonutti, Gauthier Gras and Guang-Zhong Yang, A machine learning approach for real-time modelling of tissue deformation in image-guided neurosurgery, *Artificial Intelligence in Medicine*, **80** (2017), 39-47. https://doi.org/10.1016/j.artmed.2017.07.004

[12] Randall H. Wilson, Geometric reasoning about assembly tools, *Artificial Intelligence*, **98** (1998), no. 1-2, 237-279.
https://doi.org/10.1016/s0004-3702(97)00062-3

[13] Tong Xiao, Jingbo Zhu and Tongran Liu, Bagging and boosting statistical machine translation systems, *Artificial Intelligence*, **195** (2013), 496-527.
https://doi.org/10.1016/j.artint.2012.11.005

Received: March 4, 2018; Published: March 28, 2018