FACTA UNIVERSITATIS
Series: **Mechanical Engineering** Vol. 10, N° 1, 2012, pp. 1 - 6

MATHEMATICAL MODELING THE SURFACE ROUGHNESS DISTRIBUTION OF ARTIFICIAL CELL WALL MATERIAL

UDC 631.171 631.6

Dragan V. Petrović[1#], Zoran Dj. Golubović[2], Zora Dajić[1], Kurt W. Tomantschger[3], Rade L. Radojević[1]

[1]University of Belgrade, Faculty of Agriculture, Belgrade-Zemun, Serbia
[2]University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia
[3]TU Graz, Faculty of Technical Mathematics and Technical Physics, Graz, Austria
[#]E-mail: epetrodr@agrif.bg.ac.rs

Abstract. *The plant cell walls play an important role in defining the shape and size of the plant cell, matter flow regulation, mitigation of environmental influences and achievement of homeostasis, as well as in defense and protection against pathogens in plant tissues and organs. This paper presents an original approach to the establishment of the mathematical model based upon the former study dealing with the surface nano-roughness distribution of the model cell wall. The differential equation accompanied with the appropriate additional conditions, which describes such kind of distributions, has been formulated and presented. The developed model was tested using the already reported experimental data of an artificial cell wall, made of polysaccharides based on bacterial cellulose supplemented with xyloglucan and pectin (BCPX) that imitate properties of the natural cell wall. It has been demonstrated that proposed differential equation, has an analytical solution in the form of the normal Gaussian distribution, which describes the surface roughness of cell walls made of this material accurately.*

Key words: *Nano-roughness, Mathematical model, Cell wall*

1. INTRODUCTION

Recent developments of technology have enabled the introduction of advanced digital image techniques related to the plant tissues analysis, simulation and modeling up to the smallest cell scales [3, 5, 13]. Cell walls are the major components of plant tissue. They provide for the most significant difference between plant cells and other eukaryotic cells.

Received February 21, 2012

[*] **Acknowledgement**. This research was supported by the Serbian Ministry of Science and Technological Development – projects *Improvement of biotechnological procedures as a function of rational utilization of energy, agricultural products productivity and quality increase* (Project no. TR 31051), and *Dynamical stability and instability of mechanical systems exposed to stochastically disturbances* (Project no. OI 174011).

The most abundant cell type in all plant parts is the parenchyma. Geometrical dimensions of parenchyma cells are very small and the cell wall structure analysis requires the use of different microscope techniques that allow observation at a nano-scale.

An alternative in studying mechanical cell wall properties is setting up a model of an artificial cell wall consisting of polysaccharides which imitate properties of the natural cell wall [1]. An artificial cell wall is composed of artificial parts and is an emerging technology. Polysaccharides as polymeric carbohydrate structures are formed of repeating units of mono- or disaccharides joined together by glycoside bonds. The polysaccharides structures are often linear, but may contain various degrees of branching. They can be often quite heterogeneous, containing slight modifications of the repeating unit. These macromolecules can have distinct properties in the structure from their monosaccharide building blocks. Polysaccharides can be amorphous or even insoluble in water. Polysaccharides network, based on bacterial cellulose supplemented with xyloglucan and pectin, can be used as the model cell wall [2, 14].

Cybulska et al. [4] verified the applicability of the artificial cell walls, made of polysaccharides based on BCPX, for modeling the natural cell walls. Using the atomic force microscope (AFM) topography, they provided for useful experimental source data related to the surface nano-roughness of primary cell walls and found very similar artificial structure of BCPX to the structure of the natural cell walls. Their report was a motive for the present study, focused on formulating an appropriate mathematical model of the surface nano-roughness distribution of artificial cell walls made of BCPX. Advancing the models of this kind will help in the future development of food and biopharmaceutical industry.

2. Material and Methods

The mathematical model was tested and verified using the experimental height distribution of the surface roughness elements of artificial cell wall, given in Cybulska et al. [4]. Each height class of this histogram (of m classes in total) is represented by absolute frequency n_i (i = 1,2,…, m) and appropriate interval of Δh in with, having midpoint value h_i, (i = 1, 2,…, m). Obviously, the sum of absolute frequencies equals the total samples number, i.e., $n = \sum_{i=1}^{m} n_i$.

The relative frequency (or simply frequency) of surface roughness elements of different heights, having the representative height h_i (i-th height class), is:

$$f_i = \frac{n_i}{n}, \ (i = 1,2,\ldots, m). \quad (1)$$

However, it can be also expressed in % (f_i%), by multiplying the Equation 1 by 100%.

On the base of these frequencies, common statistic parameters are evaluated: the mean, root-mean-square value (standard deviation), coefficient of variation, skewness and flatness factors [8]. In addition, the empirical probability density function (*pdf* in further text) of the nano-roughness heights of artificial cell wall made of BCPX was established using formula:

$$pdf(h_i) = \frac{f_i\%}{\Delta h} \ ; \ (i=1,2,\ldots,m). \quad (2)$$

Finally, Gaussian (normal) function

$$y = y_0 + \frac{A}{w\sqrt{\frac{\pi}{2}}} e^{-2\frac{(x-x_c)^2}{w^2}}, \tag{3}$$

is used in this paper, for analytical approximation of the surface roughness height distribution (more precisely of the empirical *pdf* in Equation 2) that characterize an artificial cell walls made by BCPX. Four fitting constants of this model function, y_0, x_C, w and A (the "center", "width", "offset" and multiplication factor, respectively) were calculated using the least-square fitting method [6, 9, 10, 12].

The accuracy of data fitting was estimated by the *root mean square error*, or so-called *standard error of estimate*:

$$RMS_E = \sqrt{\frac{\sum_{i=1}^{m}\left(y_i - \hat{y}_i\right)^2}{m-k}} . \tag{4}$$

It is based on the sum of squares of differences between the true (measured) values y_i, with respect to fitted (predicted) values y_i (i = 1, 2,..., m), where m is the number of fitted data "points" (i.e. the height classes) and k is the number of fitting constants of a model function. In general, the smaller values of RMS_E mean a higher fitting accuracy. In addition, *coefficient of determination*, or the so-called *R-square factor*:

$$R^2 = 1 - \frac{\sum_{i=1}^{l}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{l}(y_i - \overline{y})^2}, \tag{5}$$

where $\overline{y}$ was also applied to evaluate the fitting quality. The closer the value of R^2 is to 1, it means a better fitting.

Data fitting procedure, explained in this chapter, has been performed using the software package "R" [7].

3. Results and Discussion

Mathematical model

The problem under consideration can be described by the following partial differential equation of the second order:

$$\frac{\partial y}{\partial t} = \frac{w^2}{8}\frac{\partial^2 y}{\partial x^2}, \tag{6}$$

where $y = y(x,t)$ is a function which describes the height of the structural elements. Variables x *and* $t > 0$ are the coordinates of space and time, respectively, and w is a known constant.

A solution of Equation 6 is assumed in the form

$$y = t^{-\alpha} f[(x - x_c)t^{-\alpha}], \tag{7}$$

where α is an unknown constant that should be determined. Function $f(x)$ can be expressed in the form

$$f(x) = B \quad e^{-g(x)}. \tag{8}$$

Unknown function $g(x)$ has continual derivatives of the adequate order and satisfies $g(x_c) = 0$. Simultaneously, $g(x)$ and unknown constant B obey the normalization condition:

$$B\int_{-\infty}^{+\infty} e^{-g(x)}dx = 1. \tag{9}$$

Furthermore, the scaling condition

$$g(xt^{-\alpha}) = g(x)t^{-1} \tag{10}$$

holds. Using Equations 7,8 and 10, $y(x,t)$ must be given by:

$$y = Bt^{-\alpha}e^{-g(x)t^{-1}}. \tag{11}$$

Inserting this in Equation 6 implies the nonlinear differential equation

$$tg''-g'^2+\frac{8}{w^2}g = \frac{8\ \alpha}{w^2}t, \quad g = g(x), \tag{12}$$

which is satisfied by

$$g(x) = \frac{2}{w^2}(x-x_c)^2, \text{ with } \alpha = \frac{1}{2}. \tag{13}$$

So, Equation 11 becomes

$$y(x,t) = B \quad t^{-\frac{1}{2}} {}^{-\frac{2\,(x-x_c)^2}{w^2\,t}} \qquad t > 0. \tag{14}$$

Substituting Equation 14 in Equation 9 implies

$$B = \frac{1}{w}\left(\frac{\pi}{2}\right)^{-\frac{1}{2}} \tag{15}$$

Equations 14 and 15 represent the solution of Equation 6 in the form

$$y(x,t) = \frac{1}{w\sqrt{\frac{\pi}{2}}}t^{-\frac{1}{2}}e^{-\frac{2\,(x-x_c)^2}{w^2t}}. \tag{16}$$

After replacing the term $\frac{y-y_0}{A}$ in Equation 4, by new y, and taking $t = 1$ in Equation 16, equations 4 and 16 become identical.

Verification of the partial differential equation model

The analytical approximation of empirical *pdf* of the surface roughness of artificial (BCPX) cell walls is illustrated in Fig. 1 by a thick red line, while the fitting residuals are represented by a thin black line. As it can be seen in Fig. 1, this kind of distribution can be accurately described by normal function (Equation 3). This is verified by the *R-square* factor having value of 0.996 and the small root-mean square error RMS_E of 0.0363. Having in mind that normal function (Equation 3) is the solution of the partial differential Equation 6, the mathematical model is numerically verified on the base of existing experimental data.

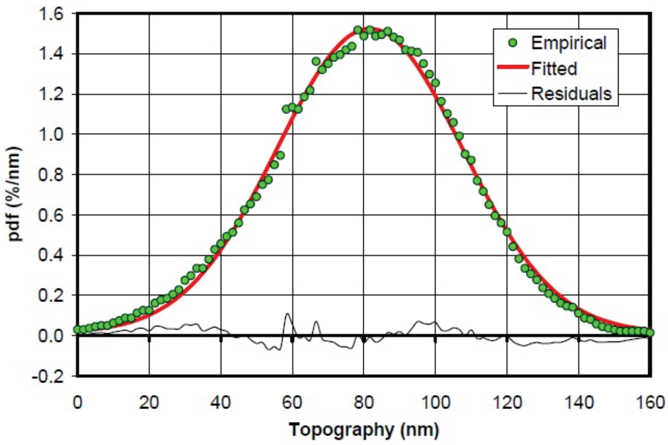

Fig. 1 Fitting results of the wall surface topography of artificial cells made by Cybulska et al. (4). LEGEND: fit line, residuals and • empirical data.

The fitting coefficients are presented in Table 1, together with the standard errors of their estimation.

Table 1 Fitting constants of Gaussian model function describing the surface topography of artificial cell walls made by Cybulska et al. (4).

Parameter	Value	Standard error
y_0	0.013070	0.00887
x_c	81.65800	0.16756
w	51.76233	0.53242
A	98.06554	1.32408

4. Conclusion

The paper presents results of studing the cell wall surface nano-roughness, based on artificial material – BCPX. The appropriate mathematical model, comprehending the partial differential equation with corresponding mathematical conditions, was formulated and presented. It is shown that the solution of this differential equation is the Gaussian function. Its applicability in approximating the surface roughness distribution of the artificial material BCPX, as a model material for apple fruit cell walls, is finally verified: an appropriate analytical form of the Gaussian function, describing the surface roughness of artificial cell walls, has been accurately found by a least-square fitting. The general advantage of approximating an experimentally determined *pdf*-s with an analytic function of suitable shape is to characterize a large amount of information, included in the empirical distribution, with an analytical function based on small number of so-called fitting constants. Presented approach facilitates sophisticated analysis and modeling of the plant texture and other properties. Future advancing the models of this kind will contribute development of the food and biopharmaceutical industry, among others.

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MATEMATIČKO MODELIRANJE RASPODELE POVRŠINSKE HRAPAVOSTI VEŠTAČKOG ĆELIJSKOG ZIDA

Dragan V. Petrović, Zoran Dj. Golubović, Zora Dajić, Kurt W. Tomantschger, Rade L. Radojević

Ćelijski zidovi biljaka imaju značajnu ulogu u definisanju oblika i veličina biljnih ćelija, kao i regulaciji razmene materija, zaštiti ćelijskih tkiva i organa od patogenih klica, ublažavanje nepovoljnih uticaja okoline itd. U ovom radu je prikazan originalni pristup formiranju matematičkog modela za opisivanje raspodele površinske nano-hrapavosti veštačkog modela ćelijskog zida. Formulisana je diferencijalna jednačina sa odgovarajućim dodatnim uslovima, koja opisuje raspodele navedenog tipa Razvijeni model je testiran koristeći postojeće (objavljene) eksperimentalne podatke merenja površinske hrapavosti veštačkih model-materijala ćelijskih zidova, izrađenih od polisaharida zasnovanih na bakterijskoj celulozi oplemenjenoj ksiloglukanom i pektinom (BCPX), koji imitira svojstva prirodnih ćelijskih zidova. Potvrđeno je da predložena diferencijalna jednačina ima analitičko rešenje u formi Gausove funkcije, koja precizno opisuje hrapavost ćelijskih zidova napravljenih od ovog materijala.

Ključne reči: *nano-hrapavost, matematički model, ćelijski zid*