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Modeling of the milling process dynamics of the fibrous semiproducts

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Abstract. Presentation of the milling as mechanochemical process allows to present a mathematical model based on the principals of formal kinetics that forms a complete mathematical description of the dynamics of the milling of fibrous semiproducts.

1. Introduction

The term “mechanochemistry” has been first introduced by Ostvald in “The book of chemistry”, where he described different methods of the initialization of the chemical processes [1]. This term can also be applied to the reactions initialized by any sort of mechanical processing. The directions of the current research can be subdivided into the investigation of the influence of the mechanical pre-processing on the reactivity capability, so-called mechanical activation, and the study of these mechanically-instigated reactions themselves, so-called mechanosynthesis [2].

The milling of the cellulose semiproducts is a mechanical process in which the cellulose fibers are split and sliced in the aqueous solution. The goal of milling is to structurally change the cell wall of the fiber via mechanical force and plasticizing effect of the aqueous solution. One of the main effects of the cellulose milling lies in “opening” the inner structure of the fibers. Cellulose fibers are flattened and become more flexible which makes them more prone to creating inter-fiber bonds [3-4].

2. Stages of the milling process

During the milling process, the mechanical process causes the shredding of the fibers and thus determine the paper structure, while the colloid physical processes resulting from the interaction of the cellulose and water determine the bonds of the fibers in the paper. The milling of the cellulose fibers can be subdivided into four stages [3-6].

First stage – the destruction of the inter-fiber connection in the cell wall and the formation of the microcracks in the wall fiber structure. Water slips through these microcracks and interacts with the free hydroxyl groups of the cellulose complex. The wedging effect of water causes the deeper splitting of the cell wall during the milling process, providing for the increase in the cellulose fibers’ flexibility and plasticity.

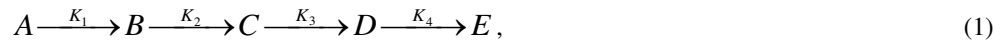


Second stage – partial destruction of the outer S1 layer and secondary S2 layer and its subsequent delamination along with primary wall P. Third stage – the swelling of the S2 wall and the formation of the structural change zones in the fibers. This process can only start after the destruction of the outer layer S1.

Fourth stage – partial destruction of the hydrogen bonds between the fibrils of the S2 wall (outer fibrillation) and the rapid growth of the fiber unit surface and water content [5-8].

3. Methods and results

This way, milling can be regarded as mechanochemical process that can be classified as mechanical activation that results in the cellulose surface preparation to the inter-fiber bond formation that helps fibers to bind into a durable paper. Based on the assumption of the milling being mechanochemical process, the dynamics of the milling can be written as:



That, like in formal kinetics, can be represented by a system of differential equations modeling the milling dynamics. A, B, C, D, and E correspond to the stages of the fiber transformation at a particular point during the process:

$$\begin{aligned} \frac{dA}{dt} &= -K_1 A \\ \frac{dB}{dt} &= K_1 A - K_2 B \\ \frac{dC}{dt} &= K_2 B - K_3 C \\ \frac{dD}{dt} &= K_3 C - K_4 D \\ \frac{dE}{dt} &= K_4 D \end{aligned} \quad , \quad (2)$$

The initial conditions are:

$$A(0)=A_0; B(0)=0; C(0)=0; D(0)=0; E(0)=0.$$

It is a system of linear differential equations with the constant factors and has a standard solution:

$$A(t) = A_0 e^{-k_1 t}, \quad (3)$$

$$B(t) = \left(-\frac{A_0 k_1 e^{-t(k_1 - k_2)}}{k_1 - k_2} + B_0 \right) e^{-k_2 t}, \quad (4)$$

$$C(t) = \left(-\frac{k_2 \left(\frac{A_0 k_1 e^{-t(k_1 - k_3)}}{-k_1 + k_3} - \frac{B_0 k_1 e^{-t(k_2 - k_3)}}{-k_2 + k_3} + \frac{B_0 k_2 e^{-t(k_2 - k_3)}}{-k_2 + k_3} \right)}{k_1 - k_2} + C_0 \right) e^{-k_3 t}, \quad (5)$$

$$\begin{aligned} D(t) = & \left(\frac{1}{(k_1 - k_3)(k_2 - k_3)(k_1 - k_3)} (-k_3 \left(-\frac{C_0(k_1 - k_2)(k_1 - k_3)(k_2 - k_3)e^{-t(k_3 - k_4)}}{-k_3 + k_4} + \right. \right. \\ & \left. \left. + k_2 \left(\frac{B_0(k_1 - k_3)(k_1 - k_2)e^{-t(k_2 - k_4)}}{-k_2 + k_4} - \frac{A_0 k_1(k_2 - k_3)e^{-t(k_1 - k_4)}}{-k_1 + k_4} \right) \right) + D_0 \right) e^{-k_4 t} \end{aligned} \quad (6)$$

$$\begin{aligned}
E(t) = & -\frac{1}{(k3-k4)(k2-k4)(k1-k4)(k1-k3)(k2-k3)(k1-k2)} \cdot \\
& (k4(\frac{1}{k4}(D0(k1-k2)(k1-k3)(k2-k3)(k3-k4)(k2-k4)(k1-k4)e^{-k4t}) + \\
& + k3(-\frac{C0(k2-k4)(k2-k3)(k1-k4)k1-k3)(k1-k2)e^{-k3t}}{k3} + (k3-k4)e^{-k4t}) \cdot \\
& k2(\frac{B0(k1-k4)(k1-k3)(k1-k2)e^{-k2t}}{k2} - A0(k2-k4)(k2=k3)e^{-k1t}))) + E0
\end{aligned} \tag{7}$$

The experimental process usually presents the milling progress as a function of time. By assuming that the milling progress S^0 is a continuous function of the degree of fiber transformation during each stage of the milling, this function can be represented by a power series around the initial starting point S^0 :

$$S^0 = S_0^0 + r_A A + r_B B + r_C C + r_D D + r_E E + R(A, B, C, D, E). \tag{8}$$

Where $R(A, B, C, D, E)$ is a part of the series containing the powers of the independent variable above 1. In linear approximation $R(A, B, C, D, E) = 0$. In this case:

$$S^0 = Const_0 + Const_1 e^{-k1t} + Const_2 e^{-k2t} + Const_3 e^{-k3t} + Const_4 e^{-k4t}. \tag{9}$$

Here $Const_i$ is a combination of the effective constants of the milling dynamics ki for each stage of the process, initial conditions and system constants (2). Based on equation (9), the second and third terms correspond to the stages of the fiber shell destruction, and the fourth and fifth represent the stages of the surface increase and fiber hydration. Thus the model can be simplified as:

$$S^0 = a_0 + a1e^{-a2t} + a3e^{-a4t}. \tag{10}$$

Figure 1 presents the dynamics model obtained from a mill rotating with the speed of 1500 rotations/minute. Figure 2 presents the results obtained from the mill rotation with the speed or 2000 rotations/minute.

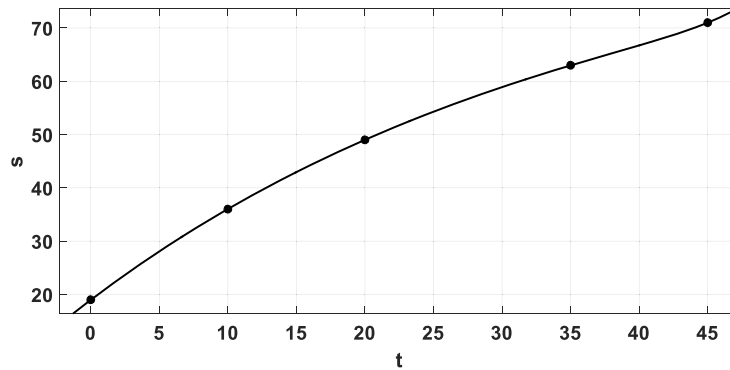


Figure 1. Model for the milling dynamics with mill speed 1500 rot/min.

General model:

$$f(x) = a_0 + a_1 e^{-a_2 x} + a_3 e^{-a_4 x}$$

Coefficients:

$$a_0=90.3; \quad a_1=1.237e-06; \quad a_2=-0.3117; \quad a_3=-71.38; \quad a_4=0.02732$$

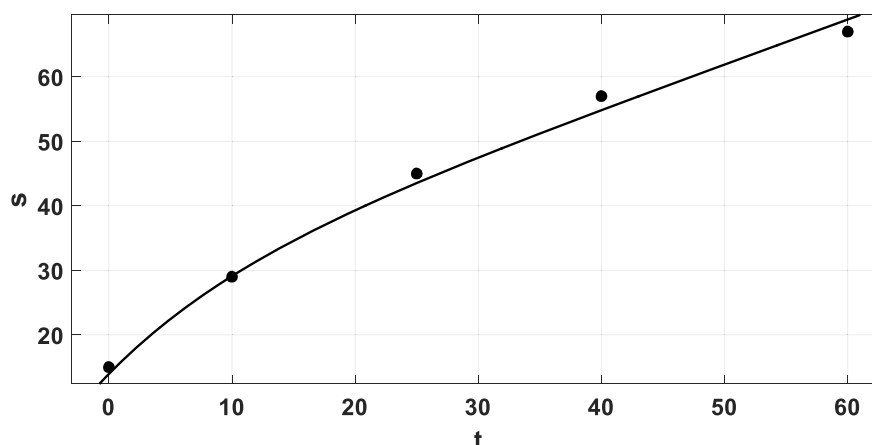


Figure 2. Model for the milling dynamics with mill speed 2000 rot/min.

General model:

$$f(x) = a_0 + a_1 e^{-a_2 x} + a_3 e^{-a_4 x}$$

Coefficients:

$$a_0=-602.8; \quad a_1=-14.75; \quad a_2=0.08802; \quad a_3=631.5; \quad a_4=-0.00103.$$

4. Conclusion

Thus representing the milling as mechanochemical process allows to model it based on the principles of the formal kinetics and present it as closed mathematical system that can be described by a system of differential equations.

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