SOFTWARE SOLUTION OF A WASHING PROCESS MATHEMATIC MODEL BY MATHEMATICA SYSTEM

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1 INTRODUCTION

The washing processes of undesirable solid calcium hydroxide from a natural polymer-hide into the washing liquid occur during the tanning operations.

The aim of deliming is to eliminate the quantity of calcium hydroxide in the processed leather. In tannery deliming operation is made during two in successive executed steps. First the occuring unbound calcium hydroxide contained in hide material is washed out from hide and second the calcium hydroxide bound with hide material is washed out from hide too.

We present the software application of the removed calcium hydroxide concentration field in the solid phase calculation during the washing process in pure bath washing. The concentration field is calculated and modelled from an analytic solution of the initial boundary problem with equation of diffusion. We visualized the derived dependence of the calcium hydroxide concentration field in the natural polymer on the space and time variable.

2 THEORY AND FORMULATION OF THE PROBLEM

In deliming washing process, the solid phase – a natural polymer is put into the washing liquid – water. Let us consider, for simplification that washed calcium hydroxide content in natural polymer is lower than its solubility in the same volume of clean water at the given temperature and also the influence of flanges on diffusion inside of the natural polymer sample is neglectable.

Besides we suppose that the washed calcium hydroxide is strong bound to the natural polymer and the washed calcium hydroxide is very well soluble during washing process. Under above mentioned assumptions we can formulate one-dimensional space-model of pure bath washing of natural polymer sample by diffusion model of calcium hydroxide concentration field inside of the natural polymer sample. The model is defined by means of partial differential equation (1) of parabolic type with following

additional conditions. The conditions ensure existence and unicity of solution of the undermentioned problem.
The solution of model is given by the field of concentration $c(x, y)$ of calcium on half-stripe domain $G = \{(x, t) \in \mathbf{R} \times \mathbf{R}^+ \mid 0 \le x \le b,\ t > 0\}$. We want to find the function $c(x,t)$ which satisfies the initial boundary problem

$$D \frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial t} + \frac{\partial c_A}{\partial t} \tag{1}$$

$$c_A = \frac{Ac}{Bc + 1} \tag{2}$$

$$c(x, 0) = c_p \tag{3}$$

$$\frac{\partial c}{\partial x}(0, t) = 0 \tag{4}$$

$$c(b, t) = \varepsilon \cdot c_0(t) \tag{5}$$

$$\frac{\partial c}{\partial x}(b, t) = -\frac{V_0}{D \cdot S} \cdot \frac{\mathrm{d} c_0}{\mathrm{d} t}(t) \tag{6}$$

$$c_0(0) = 0 \,. \tag{7}$$

V	volume of solid phase (i.e. natural polymer sample) in washing equipment	m^3
V_0	volume of washing water as a deliming reagent in washing equipment	m^3
t	time	s
c	volume concentration $Ca(OH)_2$ in natural polymer	$kg \cdot m^{-3}$
c_0	volume concentration $Ca(OH)_2$ in bath	$kg \cdot m^{-3}$
c_p	initial concentration $Ca(OH)_2$ in natural polymer	$kg \cdot m^{-3}$
D	effective diffusion coefficients of washed calcium hydroxide out from natural polymer	$m^2 \cdot s^{-1}$
D^*	modified diffusion coefficient (of bath washing)	$m^2 \cdot s^{-1}$
x	position coordinate	m
b	half thickness of natural polymer	m
ε	porosity (ratio of poroses volume to natural polymer sample volume)	1
Na	soak number (ratio V_0 / V)	1
q_n	n-th root of a certain transcendent equation	1
A	sorption balance constant (from Langmuir's sorption isotherm)	1
B	sorption balance constant (from Langmuir's sorption isotherm)	$m^3 \cdot kg^{-1}$
S	from one-side area of natural polymer	m^2
F_o	Fourier criterium (dimensionless time)	1
C	dimensionless volume concentration $Ca(OH)_2$ in natural polymer	1
C_0	dimensionless volume concentration $Ca(OH)_2$ in bath	1
X	dimensionless space coordinate	1

Tab. 1: List of symbols

The quation (1) describes the washed calcium hydroxide out from a natural polymer sample in the direction of water bath. The last term on the right side of equation (1) depends on desorption mechanism of washed calcium hydroxide out from solid phase. Suppose that diffusion is determining for change rate of concentration, it is possible to express the dependence of c_A (of fixed calcium hydroxide) on the free calcium hydroxide c by relation of Langmuir's sorption isotherm (2). Condition (3) shows initial distribution of concentration in solid phase. Boundary condition (4) denotes that field of concentration in solid phase is symmetric.

Relation (5) holds under condition of a perfectly mixed liquid phase. Balance condition (6) denotes the equality of the diffusion flux at the boundary between the solid and liquid phases with the speed of accumulation of the diffusing element in the surrounding. Relation (7) describes that we use clean water for natural polymer bath washing.

Suppose that considered concentration $c(x, t)$ of calcium is very low, i.e. $Bc << 1$, we can define domain in which sorption isotherm comes into the linear form and thus relation (2) will be in more simple form

$$c_A = A \cdot c \tag{8}$$

and system of equations will be in linear form

$$\frac{\partial c}{\partial t} - D^* \frac{\partial^2 c}{\partial x^2} = 0, \quad \text{where constant } D^* = \frac{D}{A+1}. \tag{9}$$

For high concentrations, when $Bc >> 1$, we obtain $c_A = A/B$ for high values, which is a maximum of sorbed calcium hydroxide concentration. For simplification of solution of equation (9) with additional conditions (3–7) we introduce dimensionless variables

$$C = \frac{c}{c_p}, \quad C_0 = \frac{c_0}{c_p}, \quad F_o = \frac{D t}{b^2 (A+1)}, \quad X = \frac{x}{b}, \quad Na = \frac{V_0}{V}.$$

By means of Laplace transformation we obtain analytic solution. Final solution given by dimensionless concentration field $C(X, F_o)$ can be expressed as follows

$$C(X, F_o) = \frac{\varepsilon (A+1)}{\varepsilon (A+1) + Na} - 2\, Na \cdot \sum_{n=1}^{\infty} \frac{\cos(q_n X) \exp\left(-q_n^2 F_o\right)}{\varepsilon (A+1) \cos(q_n) - \dfrac{\varepsilon (A+1)}{q_n} \sin(q_n) - Na \cdot q_n \sin(q_n)}, \tag{10}$$

where q_n is the n-th positive root of the following transcendent equation

$$\tan q + \frac{V_0}{(A+1) V \varepsilon} \cdot q = 0 \tag{11}$$

which is solved numerically.

3 SOFTWARE SOLUTION OF THE PROBLEM

We show the software solution for calculation and visualization of concentration field in solid phase of washed bound calcium hydroxide by means of the computer algebraic system Mathematica.

The dimensionless concentration fields in natural polymer can be calculated and displayed for one (position) or two (position and time) variables (see Fig. 1). We used equation (10) for computation of the dimensionless concentration field. Furthermore, the software application can calculate the values of washed calcium hydroxide concentration in a given time and a place of the natural polymer too.

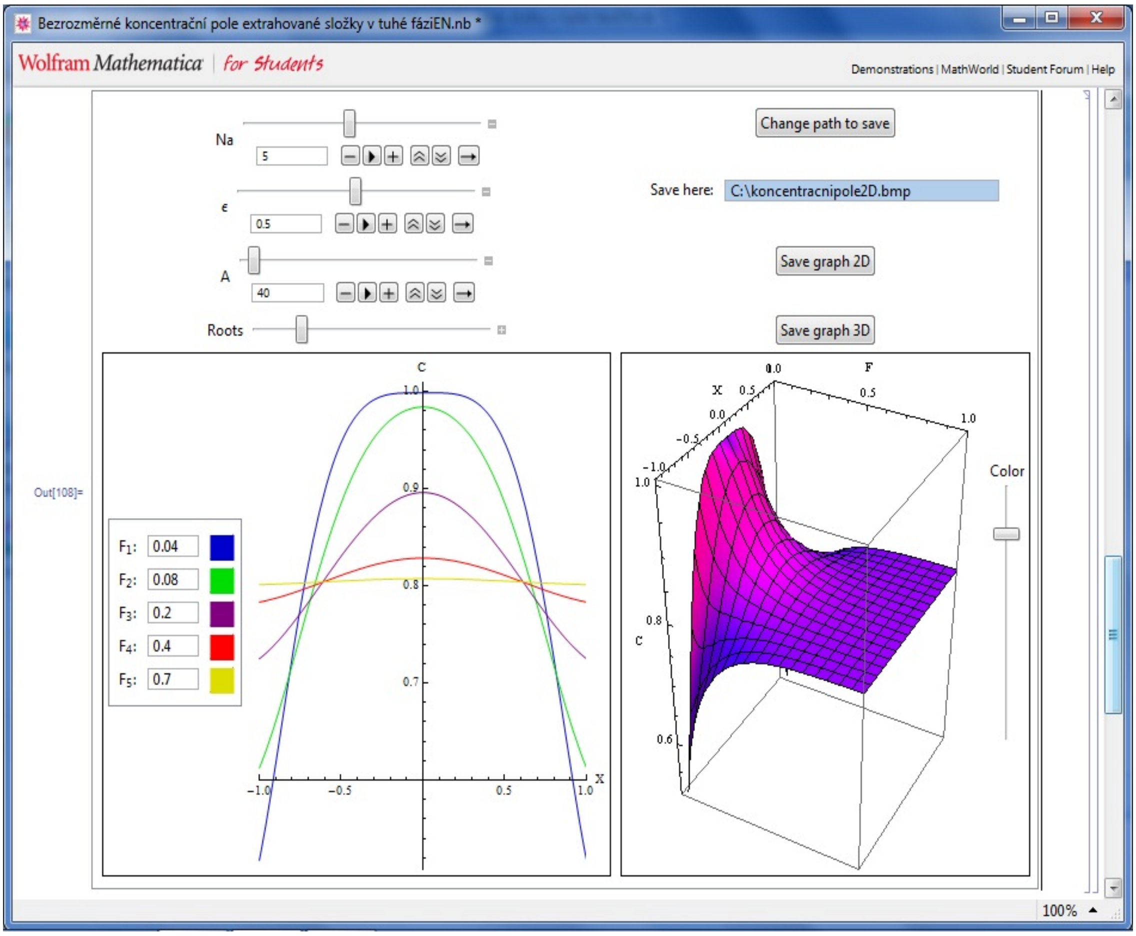

Fig. 1

CONCLUSION

The previous experience with mathematic modelling and its graphic outputs proves that together with 3D graphics the usefulness of 2D graphics will not be decreasing.

Presented software application enables us to effectively evaluate the influence of input parameters on the output parameters in studied calcium hydroxide concentration field model of pure washing process. It enables us to utilize that acquired data for more complex mathematic models, e.g. for models of the chemical bath washing by the chemical agents in tannery, and thus optimize the main industrial processes in tanning industry in light of the operating costs and also with regard to the ecological point of view.

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