TREATMENT OF THE INDIRECT MODELLING OF A DIFFUSION PROCESS IN A FLOW SYSTEM WITH THE RETENTION BY MAPLE SYSTEM

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1 Introduction

An extraction process of undesirable components from a solid material by using of an extraction liquid is very often used during the nature polymers processing. For propose of an optimal course of these components extraction, the physico-chemical formulation of the process is necessary to know. The proposal can be determined by both experimentally or appropriate mathematical model solving. The operation time course is often hardly experimental determined and in addition time-consuming. Therefore, it is advantageous to use the second above mentioned proposed procedure, i.e. the mathematical model to suggest.

In the contribution we deal with creation of the software application of the removed component concentration field in the solid phase calculation during the extraction process in flow system with retention. The calculation is based on analytical solution of the extraction process mathematical model. We visualized the derived dependence of the removing component concentration for dimensionless variables in the solid phase on the operating time.

2 MATHEMATICAL MODEL OF THE EXTRACTION PROCESS IN FLOW SYSTEM WITH RETENTION

We discuse the mathematic formulation of the problem in paper [1] in detail. If we suppose that the extracted component is strong bound to the solid material

and the extracted component is very well soluble during extraction process the mathematical model can be described by the following equations (1) – (7)

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

$$c(x,0) = c_p \tag{2}$$

$$c_0(0) = 0 \tag{3}$$

$$c(b,t) = \varepsilon \cdot c_0(t) \tag{4}$$

$$\frac{\partial c}{\partial x}(0,t) = 0 \tag{5}$$

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

We introduce dimensionless variables for the solution of equation (8) with additional conditions (1 – 6)

$$C = \frac{c}{c_p}, \quad C_0 = \frac{c_0}{c_p}, \quad F_o = \frac{D \cdot t}{b^2 \cdot (1+A)}, \quad X = \frac{x}{b}, \quad Na = \frac{V_0}{V}, \quad L = \frac{Q_V \cdot b^2}{D^* \cdot V_0}. \tag{7}$$

By means of Laplace transformation we obtain analytic solution. Final solution given by dimensionless concentration field $C(X, F_o)$ in solid phase holds

$$C(X,F_o) = 2\sum_{n=1}^{\infty} \frac{[DV_0 q_n^2 - (1+A)Q_V b^2]\mathrm{e}^{-q_n^2 \cdot Fo} \cos(q_n \cdot X)}{q_n [DV_0 q_n (q_n \sin q_n - 2\cos q_n) - (1+A)(DV\varepsilon + Q_V b^2)\sin q_n - (1+A)DV\varepsilon q_n \cos q_n]} \tag{8}$$

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

$$\tan q = \frac{(1+A)Q_V b^2 - q^2 V_0 D}{(1+A)DV\varepsilon q}. \tag{9}$$

3 THE SOFTWARE APPLICATION

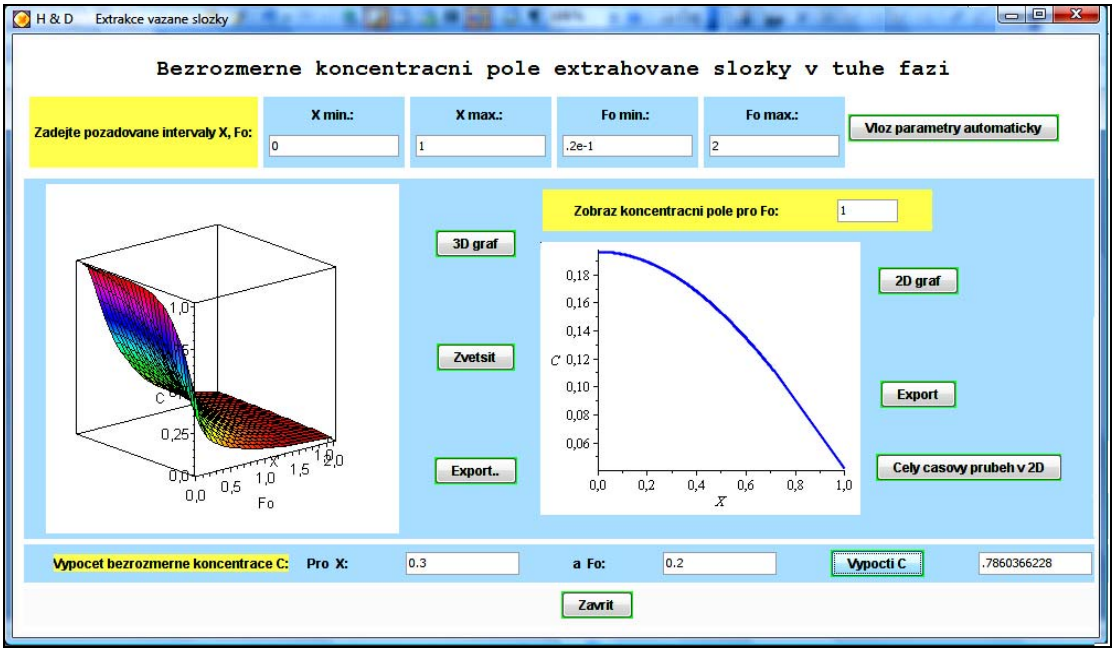

FIG. 1 Window for solving and visualization of dimensionless concentration field in solid phase

We made up the software application for calculation and visualization of extracted bound component concentration field in solid phase in the computer algebraic system Maple. Our calculation consists of two basic parts. Firstly the positive roots q have to be numerically solved for input parameters from equation (9).

Subsequently, dimensionless concentration fields can be calculated and displayed for one or two variables (see Fig. 1). We used equation (9) for computation of the dimensionless concentration field. The obtained graphics can be viewed and exported to postscript graphic format, when appropriate (see Fig. 2, Fig. 3). Furthermore, the software application can calculate the values of extracted component concentration in a given time and a place of the solid phase too.

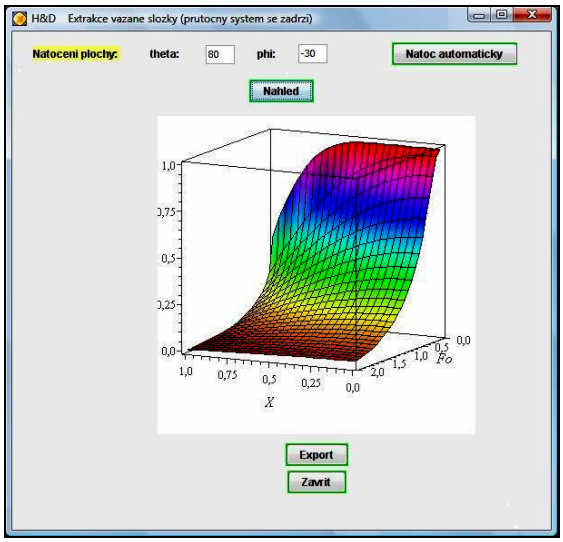

FIG. 2 Window for view and export of dimensionless concentration field in solid phase like a function of position and time

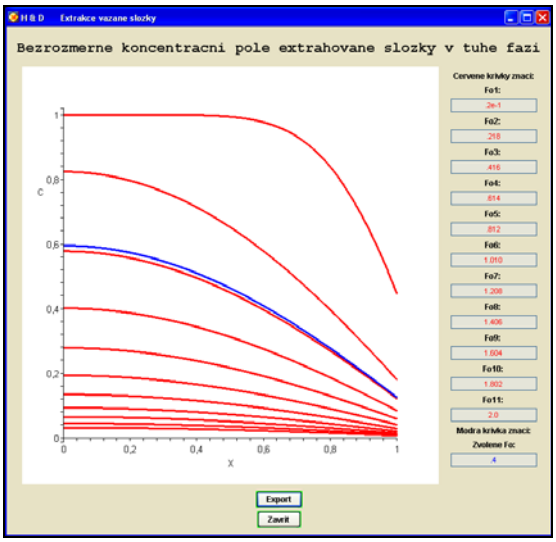

FIG. 3 Window for view and export of dimensionless concentration field in solid phase like a function of time

Table of the used symbols:

V	volume of solid phase	m^3
V_0	volume of washing water as a deliming reagent in washing equipment	m^3
Q_V	volume flow rate (the time derivative dV_0/dt)	$m^3 \cdot s^{-1}$
t	time	s
c	Extracted component volume concentration in solid phase	$kg \cdot m^{-3}$
c_0	Extracted component volume concentration in washing equipment	$kg \cdot m^{-3}$
c_p	Extracted component initial concentration in solid phase	$kg \cdot m^{-3}$
D	effective diffusion coefficients of washing component from solid phase	$m^2 \cdot s^{-1}$
D^*	modified diffusion coefficient (of washing)	$m^2 \cdot s^{-1}$
x	position coordinate	m
b	half thickness of solid phase	m
ε	porosity of solid phase	1
Na	soak number (the 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
S	area of solid phase	m^2

F_o	Fourier criterium (dimensionless time)	1
C	Extracted component dimensionless volume concentration in solid phase	1
C_0	Extracted component dimensionless volume concentration in washing equipment	1
X	dimensionless space coordinate	1
L	dimensionless flow of extraction solvent	1

CONCLUSION

The analytical solution of the mathematical model in case of the bound component extraction from the solid material to the extraction solvent during a flow washing in system with retention enabled us to make the software application for calculation and visualization of time-course of the extraction process for dimensionless variables.

The software application can be used for description of any technological process which is based on the same mechanism.

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