Diffusion Model of Washing Process

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Abstract: The paper contents the optimization of the washing processes which are characterized by large consumption of water and electrical energy mainly. For this reason is very important deal with them. For the optimization process of washing it is possible to set up an access of the indirect modeling that is based on make-up of mathematical models coming out of study of the physical operation mechanism. The process is diffusion character it is characterized by the value of diffusion effective coefficient and so called structure power of the removing item to the solid phase. The mentioned parameters belong to input data that are important for the automatic control of washing process.

Key-Words: - Mathematic modeling, optimization, wash process, washing of bound component.

1 Introduction

The purpose of the washing process is to wash out the undesirable components from solid phase by water in which the washed component is very well soluble.

It is possible to divide the washing processes into several cases according to the way of adjustment – Fig 1 [Janáčová 2003].

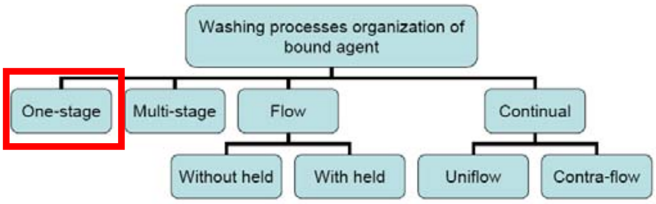

Fig.1: The cases of washing processes adjustment

The quantitative description goes from the mechanism, from the individual ways of washing process adjustment, and it is based on the weight balance of washed component.

The mechanism of the process depends on that:
-How the washed substance is bound
- Which way
- How strong

2 Theory

For next procedure of the washing process rationalization it is substantial in which part of the sorption isotherm a state of washed component can be found. Based on Fig.3 it is the state *C* or *B*. In the area of state *C* the washed component is free (does not bind), in the area B the washed component is bound to solid phase. In this area it is also possible to delimitate zone *A*, in which the sorption dependence is practically linear. The constant of proportionality (an equilibrium constant of sorption) characterizes the strength of linkage to solid phase, i.e. largely it can determine how the washing process is effective in this area.

In the simplest case it is possible to express this dependence by Langmuir sorption isotherm:

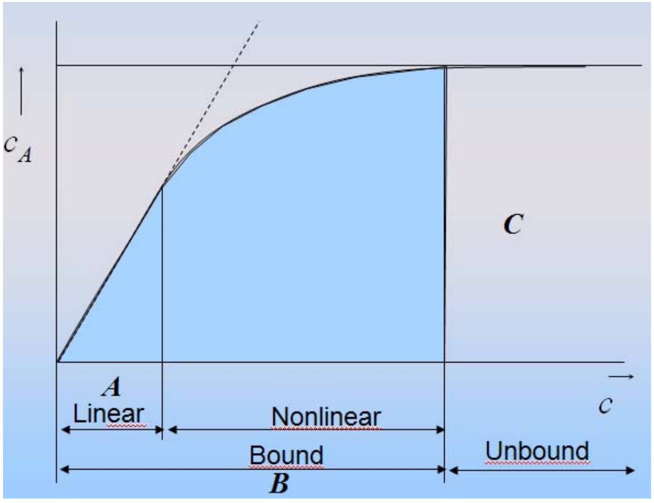

Fig.2: Langmuir´s sorption isotherm

The easiest possibility of the sorption constants setting

A, B of Langmuir isotherm is directly use of its quantification.

$$c_A = \frac{Kc}{Bc+1} \quad (1)$$

This procedure needs relatively precise setting both solid and liquid phase. However the setting of calcium ions concentration in material can cause complications. On this account was designed the indirect method only incumbent in analyse of liquid phase. To this purpose can be derived dependence

$$\frac{1}{c_S - c_0(\varepsilon + Na)} = \frac{1}{\varepsilon \cdot c_0 \cdot A} + \frac{B}{A} \quad (2)$$

from its direction is figured out sorption constant *A* and from the section at the axis of dependent variable can be determined for known constant *A* the value of sorption constant *B*.

For very small values c is possible product *B.c* in relation (1) vanish on 1, it means 1 >> *B*.c. Then can be written

$$c_A = K \cdot c \quad (3)$$

Where we set off the exact value of constant *A* on nonlinear relation (1) and approached it by constant value *K*, from linear relation (3), it means that here valid:

$$K \approx A \quad (4)$$

By the modification will get an appropriate quadratics for the estimation of sorption constant *K*, let us say *A*

$$C_0^* = \frac{c_S}{c_0} = \varepsilon\,(K+1) + Na \quad (5)$$

Mathematical model of the one-stage washing

In this process, the material is put into the washing liquid. The washing liquid flows neither in nor out of the bath. Under assumptions that calcium hydroxide content in material is lower than its solubility in the same volume of washing liquid at the given temperature and the influence of flanges on diffusion inside of the material sample is neglectable can formulate one-dimensional space-model of bath washing of material sample by diffusion model of transport of washed out calcium hydroxide

$$\frac{D}{A+1} \cdot \frac{\partial^2 c(x,t)}{\partial x^2} = \frac{\partial c(x,t)}{\partial t}, \; t > 0, \quad 0 \le x \le b \quad (6)$$

$$\frac{\partial c}{\partial x}(b,t) = -\frac{V_0}{D \cdot S} \cdot \frac{\mathrm{d}c_0}{\mathrm{d}t}(t) \quad (7)$$

$$c(x,0) = c_p \quad (8)$$

$$c_0(0) = 0 \quad (9)$$

$$\frac{\partial c}{\partial x}(0,t) = 0 \quad (10)$$

$$c(b,t) = \varepsilon \cdot c_0(t), \quad (11) \qquad \text{where } c_A = \frac{Kc}{Bc+1}$$

Equation (6) represents component ions diffusion from material in the direction of washing liquid bath. The expression of the right hand side last term of equation depends on desorption mechanism of washing component from solid phase. If we suppose that diffusion is determining for change rate of concentration then it is possible to express the dependence of bound component c_A on the unbound component *c* by the relation of Langmuir's sorption isotherm (1). Condition (7) shows the initial distribution of calcium ions concentration in solid phase-material. Relation (8) describes that we use pure water for material bath washing. Relation (9) holds under condition of a perfectly mixed liquid phase. Boundary condition (10) denotes that field of concentration in solid phase is symmetric. Boundary balance condition (11) denotes the equality of the diffusion flux at the boundary between the solid and the liquid phases with the speed of accumulation of the diffusing element in the surrounding.

We introduce dimensionless variables for the solution of equation (9) with additional conditions (8,9)

$$C = \frac{c}{c_p}, \; C_0 = \frac{c_0}{c_p}, F_o = \frac{D \cdot t}{b^2 \cdot (1+A)}, X = \frac{x}{b}, \; Na = \frac{V_0}{V} \quad (12a,b,c,d,e)$$

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

$$C(X,F) = \frac{\varepsilon\,(1+A)}{\varepsilon\,(1+A) + Na} - 2\,Na \cdot \sum_{n=1}^{\infty} \frac{\cos\,(q_n\,X)\,\exp\,(-q_n^2 F)}{\varepsilon(1+A)\,\cos\,(q_n) - \frac{\varepsilon\,(1+A)}{q_n}\,\sin\,(q_n) - Na \cdot q_n \sin(q_n)} \quad (13)$$

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

$$-\frac{Na \cdot q}{\varepsilon \cdot (1+A)} = \tan(q) \quad (14)$$

3 Optimization of washing process

The analytic solution of mathematic model of bath washing process enabled us to determine the operating costs-function for bath washing of material. It is possible to find the optimum of washing water of process to be successful course of the process respectively, and that all from the corresponding the operating costs-function. To determine the operating costs-function for the material bath washing we assumed that we are able to eliminate component from the material by the water and that the main operating costs N_C of considered process are given by the sum of the consumed electric energy to the drive of machinery costs N_E and the consumed washing water costs N_V

$$N_C = N_V + N_E, \qquad (15)$$

whereas the consumed electric energy costs are given by the product of the electric power unit price K_E, the time t and the electromotor input P to the drive of machinery

$$N_E = K_E \cdot P \cdot t. \qquad (16)$$

The costs of the washing water requirements N_V are given by the product of unit price of washing water K_V and the washing water volume V_0

$$N_V = K_V \cdot V_0. \qquad (17)$$

We supposed as well that the increasing water requirements cause the decreasing of water pollution during the washing whereby the effectiveness of washing process increases. Thereby the time interval, necessary to the drive of machinery is shorter, hence the electric energy costs are decreasing because these are linearly increasing with dependence on time. This implies that the sum of the water requirements costs and the electric energy in dependence on the water requirements keeps a minimum.

If we want to determine the total costs in dependence on the total dimensionless washing water requirements then first it was necessary to determine the dependence of the washing degree y, which determines the efficiency of the washing process in dependence on the dimensionless time Fo and that for the corresponding soak number Na.

4 Simulation of washing process in software application

Mathematic description of washing process course is complicated. On the other hand, we need prompt basic information about the process course for an optimal process control. Therefore we made software application, which can calculate and graphical display bound component concentration field in solid material during washing.

We made our application in the computer algebraic system Maple, which is a comprehensive environment for exploring and applying mathematics. By using of Maple programming language, we created user interface of our application in the Maplet form.

Our application contains several windows with the specific functions. The first window is destined for definition of process conditions, and for calculation of roots q_n. The values q_n are obtained by numeric solution of equation (9).

After this calculation, the dimensionless concentration field $C(X,F_o)$ or concentration field $c(x, t)$ for real variables can be displayed. The calculation is based on solution (13) of the mathematic model, which we described in the previous section. We show window for visualization of dimensionless concentration field in the Fig. 3. The concentration field can be visualized as a surface $C(X,F_o)$ (3D graphics) or as a curve $C(X)$ (2D graphics) in specific dimensionless time F_o.

5 The software application using

We present our application using in the following example which describes bound component removing that proceeds under these conditions:

Volume of washing liquid V:	1 m^3
Volume of solid material in bath V_0:	3 m^3
Initial concentration of bound component in material c_p:	10 kg·m^{-3}
Thickness of solid material $2b$:	4 mm
Effective diffusion coefficient D:	$1\cdot10^{-8}$ m^2·s^{-1}
Porosity of solid material ε:	0.5

Fig. 4 illustrates course of washing in the solid material under above mentioned conditions. Fig. 5 shows quantitative description of the process. It provides basic information about washing. It is evident, that diffusion process proceeds from the boundary between solid material and washing liquid in the direction of solid material centre. Furthermore, the washing liquid causes a rapid decreasing of bound component concentration in solid material in a short operating time.

As you can see in Fig. 4,5 in the time between approximately 1800 and 3600 seconds, the bound component concentration decreases nearly negligible because most of bound component already diffused from the material into the washing bath. In practice, the prolonging time of process causes increasing of operating cost.

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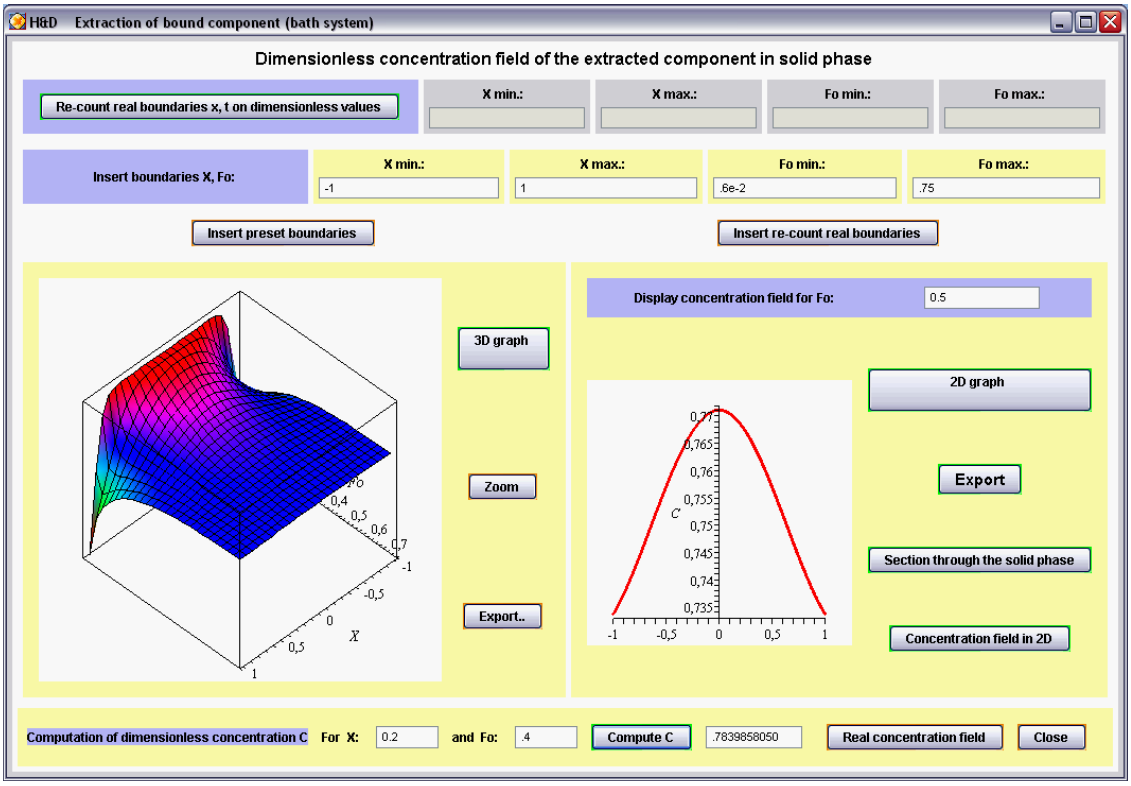

Fig. 3 Show of the window for computing of the dimensionless concentration field

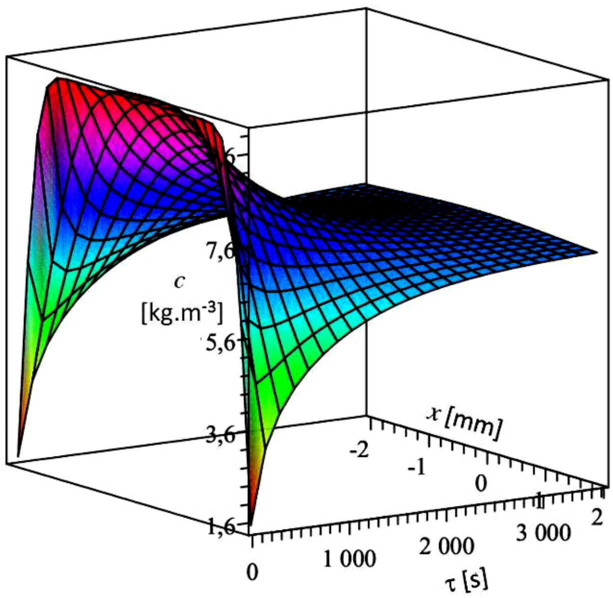

Fig. 4 Bound component concentration field in solid material $c(x, t)$ during washing

Furthermore, the bound component concentration near the surface of solid material first rapidly decreases and after them rapidly increases. In practice, the prolonging time of washing causes increasing of operating cost.

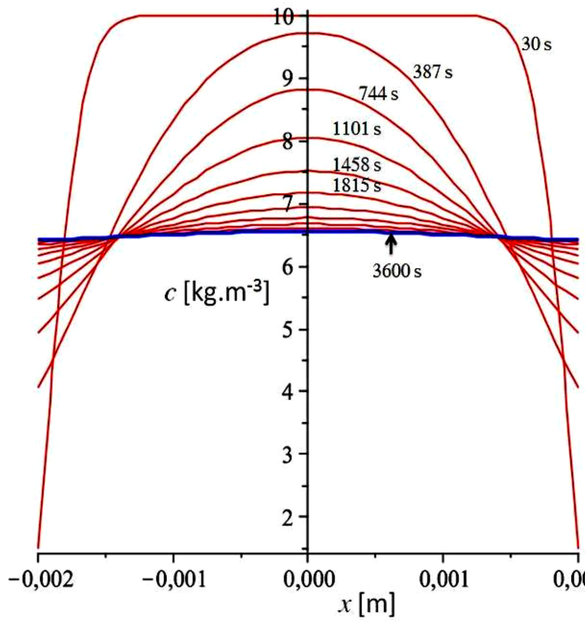

Fig. 5 Concentration field in the solid material in the specific operation time

5 Conclusion

The proposed model was employed in the optimization of component washing from solid phase. The analytical solution of mathematical model in the case of the one-cycle bound component washing from the solid material to the extraction solvent enabled us

to make the software application for calculation of the extraction process course for both real and dimensionless variables.
The application was used for determination of optimal process course.
The washing process course was also succesfuly verified by laboratory experiments for deliming process [Charvatova, 2007]. The main advantage of this work is that the optimal consumption washing from solid phase in bath system. The application will also be used for description and optimization of other

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LIST OF SYMBOLS

V	volume of solid phase (material)	m^3
V_0	volume of washing water	m^3
t	time	s
c	volume concentration of component in material	$kg \cdot m^{-3}$
c_0	volume concentration of component in bath	$kg \cdot m^{-3}$
c_p	initial concentration component in material	$kg \cdot m^{-3}$
D	effective diffusion coefficients of washing component from material	$m^2 \cdot s^{-1}$
x	position coordinate	m
b	half thickness of material	m
ε	porosity (ratio of poroses volume to materialsample volume)	1
Na	dimensionless consumption of water (ratio V_0 / V)	1
q_n	$n^{\text{-th}}$ root of a certain transcendent equation	1
A	sorption constant (from Langmuir's sorption isotherm)	1
B	sorption balance constant (from Langmuir's sorption isotherm)	$m^3 \cdot kg^{-1}$
S	area of pelt	m^2
F_o	Fourier criterium (dimensionless time)	1
C	dimensionless volume concentration component in material	1
C_0	dimensionless volume concentration component in bath	1
X	dimensionless space coordinate	1

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