Computer simulation of washing processes

D. Janáčová, H. Charvátová, K. Kolomazník, V. Vašek, P. Mokrejš and R. Drga

***Abstract*—**The paper contents the optimization of the washing processes which are characterized by large consumption of washing liquid 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 material. The mentioned parameters belong to input data that are important for the automatic control of washing process.

***Keywords*—**Mathematic modeling, optimization, wash process, washing of bound component.

I. Introduction

THE purpose of the washing process is to wash out the undesirable components from solid material by liquid 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 [1].

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 [2].

The mechanism of the process depends on that how the washed substance is bound:

- Which way
- How strong

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II. Theory

For next procedure of the washing process rationalization it is substantial in which part of the sorption isotherm a state of

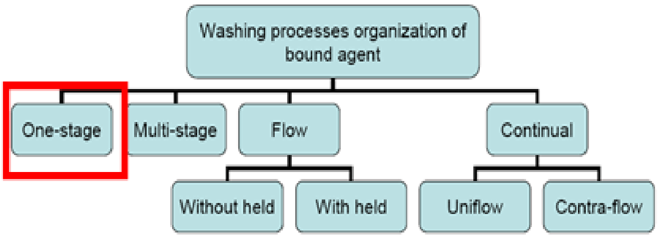

Fig. 1 The cases of washing processes adjustment

washed component can be found. Based on Fig.2 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 [3].

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

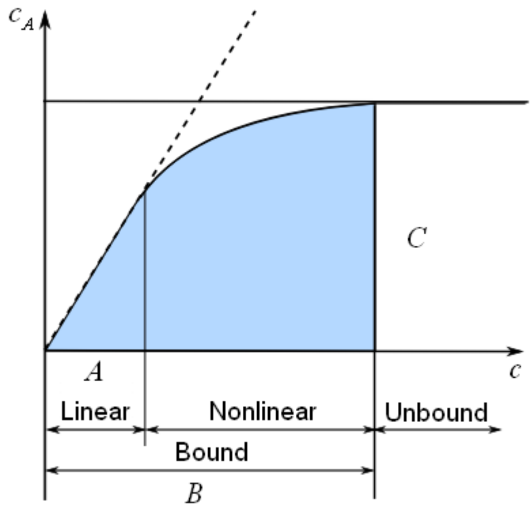

Fig. 2 Langmuir sorption isotherm

$$c_A = \frac{Kc}{Bc+1} \tag{1}$$

This procedure needs relatively precise setting both solid and liquid phase. However, the setting of washed component concentration in material can cause complications. On this account was designed the indirect method only incumbent in analyze of liquid phase. To this purpose can be derived dependence (2) [9]

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

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

For very small values c is possible product $B.c$ in equation (1), it means 1 >> $B.c$, can be written

$$c_A = K \cdot c \tag{3}$$

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:

$$K \approx A \tag{4}$$

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

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

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 (Fig. 3). Under assumptions that washed component 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 component (Fig. 3) [4], [5], [6] .

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

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

$$c(x,\ 0) = c_p \tag{8}$$

$$c_0(0) = 0 \tag{9}$$

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

$$c(b,t) = \varepsilon \cdot c_0(t) \tag{11}$$

where concentration c_A is given by equation (1).

Equation (6) represents washed component diffusion from

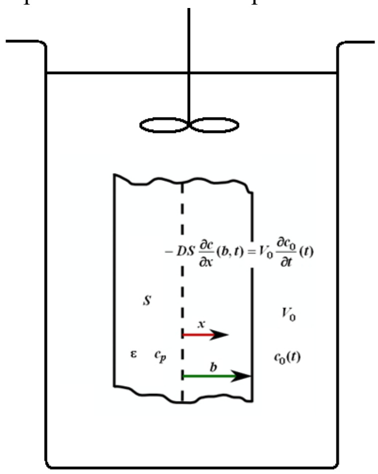

Fig. 3 Sketch of the washing process

material in the direction of washing liquid in the 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 sorption isotherm (1). Condition (8) shows the initial distribution of washed component concentration in solid phase-material. Equation (9) describes that we use pure washing liquid for material bath washing. Equation (11) holds under condition of a perfectly mixed liquid phase. Boundary condition (10) denotes that field of concentration in solid material is symmetric. Boundary balance condition (7) 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 (1), (7) - (11)

$$C = \frac{c}{c_p},\ C_0 = \frac{c_0}{c_p},\ F_0 = \frac{D \cdot t}{b^2 \cdot (1+A)},\ X = \frac{x}{b},\ Na = \frac{V_0}{V}$$

(12 a, b, c, d, e)

By means of Laplace transformation we obtained analytic solution. Final solution given by dimensionless concentration field $C(X, F_0)$ in the material [3]:

$$C(X,F_o)=\frac{\varepsilon(1+A)}{\varepsilon(1+A)+Na}$$
$$-2Na\cdot\sum_{n=1}^{\infty}\frac{\cos(q_nX)\exp(-q_n^{\,2}F_0)}{\varepsilon(1+A)\cos(q_n)-\frac{\varepsilon(1+A)}{q_n}\sin(q_n)-Na\cdot q_n\sin(q_n)} \qquad (13)$$

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

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

III. Optimization of Washing Process

The analytic solution of mathematic model of bath washing process enabled us to determine the cost function for bath washing of material. It is possible to find the optimum of washing liquid of process to be successful course of the process respectively, and that all from the corresponding the cost function [5], [7], [8].

To determine the cost function for the material bath washing we assumed that we are able to eliminate component from the material by the washing liquid and that the main processes 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 liquid 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 liquid requirements N_V are given by the product of unit price of washing liquid K_V and the washing liquid volume V_0

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

We supposed as well that the increasing washing liquid requirements cause the decreasing of washing liquid 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 washing liquid requirements costs and the electric energy in dependence on the washing liquid requirements keeps a minimum.

If we want to determine the total costs in dependence on the total dimensionless washing liquid requirements then first it is necessary to determine the dependence of the washing degree y, which determines the efficiency of the washing process in dependence on the dimensionless time F_o and that for the corresponding soak number Na. Dependence of the washing degree y, on the dimensionless time F_o is given by equation (18) [3]

$$y=\frac{C_0Na}{1+A}=$$
$$=\frac{Na}{\varepsilon\ (1+A)+Na}-2\frac{Na^2}{\varepsilon\ (1+A)}\sum_{n=1}^{\infty}\frac{\exp\left(-F_o\ q_n^{\,2}\right)}{\varepsilon\ (1+A)+\frac{q_n^{\,2}Na^2}{\varepsilon\ (1+A)}+Na} \qquad (18)$$

In the Fig. 4 is depicted dependence of the washing degree on the time. The time is computed from Fourier number according to equation (12c)

In the Fig. 5 we show detailed sketch of determination time to reaching demanded washing degree

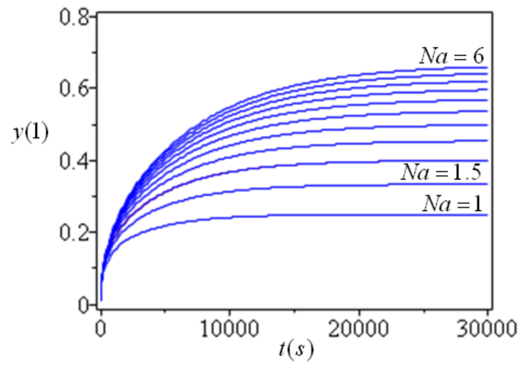

Fig. 4 Dependence of the washing degree on the time for various soak numbers
b = 0.002 m, A = 5, ε = 0.5, $D = 6\cdot10^{-9}$ m$^2\cdot$s^{-1}, c_p = 10 kg·m^{-3}

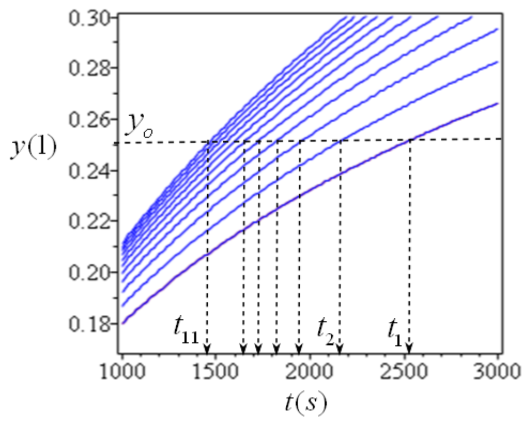

Fig. 5 Detailed sketch of determination time to reaching demanded washing degree
b = 0.002 m, A = 5, ε = 0.5, $D = 6\cdot10^{-9}$ m$^2\cdot$s^{-1}, c_p = 10 kg·m^{-3}
$Na_{min}=2$, $Na_{max}=6$

Determination of time to reaching demanded washing degree of given soak number enable to compute cost function according to equation (19)

$$N_C = K_V \cdot Na \cdot V + \frac{K_E \cdot P \cdot F_o \cdot b^2 \cdot (1+A)}{D} \qquad (19)$$

IV. Simulation of Washing Process in Software

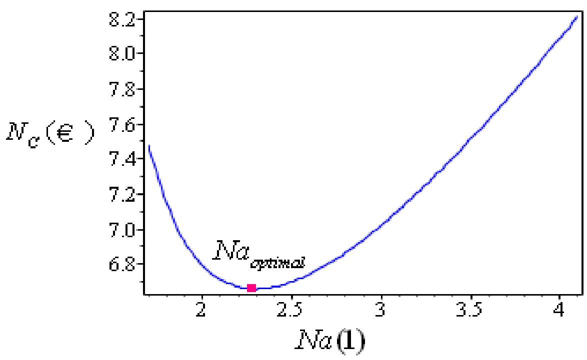

Fig. 6 Cost function - determination of the optimal soak number
$b = 0.002$ m, $A = 5$, $\varepsilon = 0.5$, $D = 6{\cdot}10^{-9}$ $m^2{\cdot}s^{-1}$,
$c_p = 10$ $kg{\cdot}m^{-3}$, $P = 10$ kWh, $K_V = 1.5$ $€{\cdot}m^{-3}$, $K_E = 0.5$ $€{\cdot}kW{\cdot}^{-1}h^{-1}$

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 (Fig. 7).

It 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 (14).

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 windows for visualization of concentration field for real values in the Fig. 8 – Fig. 10. 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.

The application can also compute cost function for required parameters of the washing process (Fig. 11, Fig. 12).

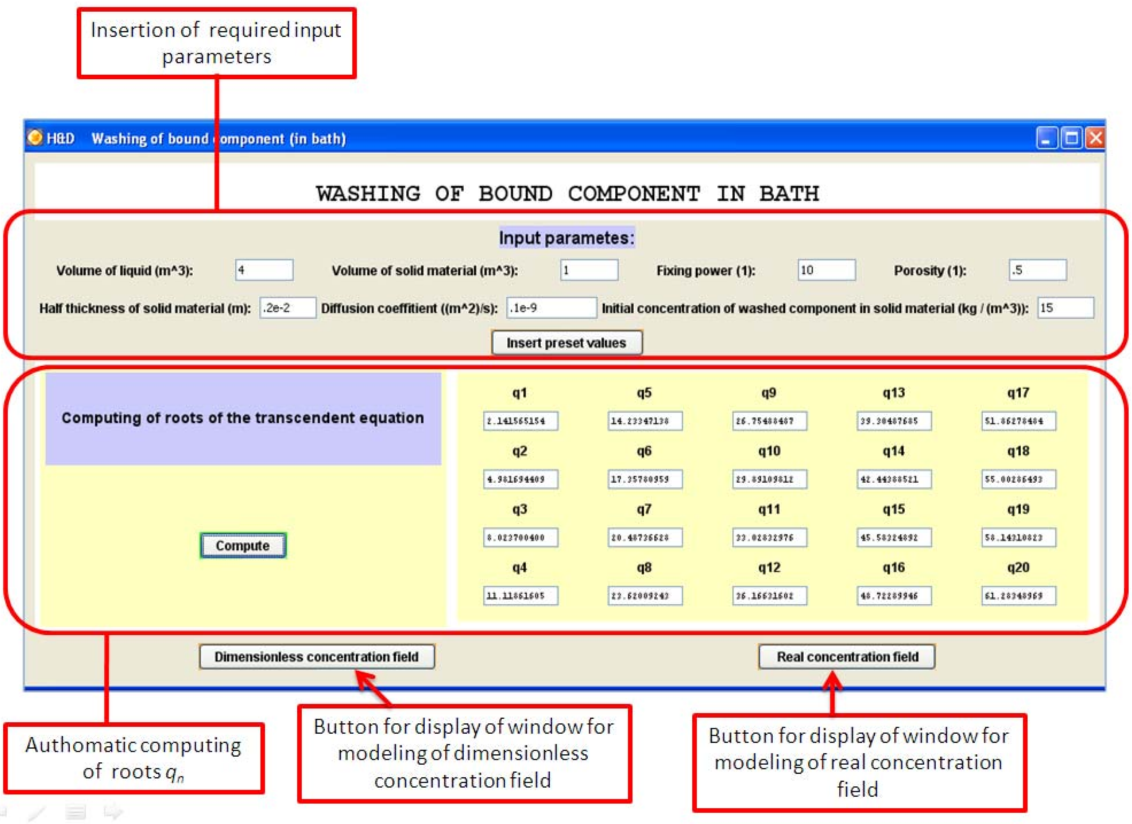

Fig. 7 Initial window of the software application

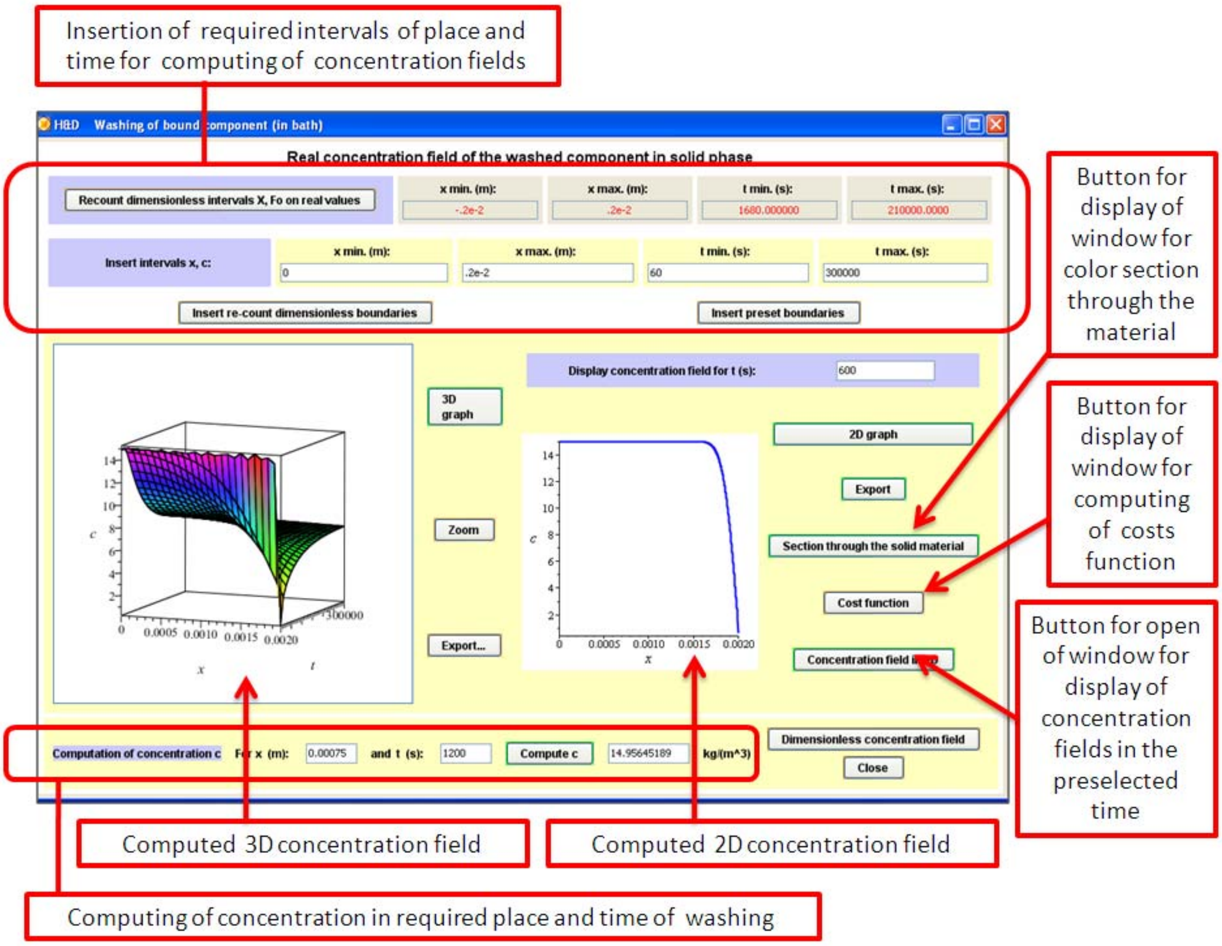

Fig. 8 Window for modeling of the real concentration field

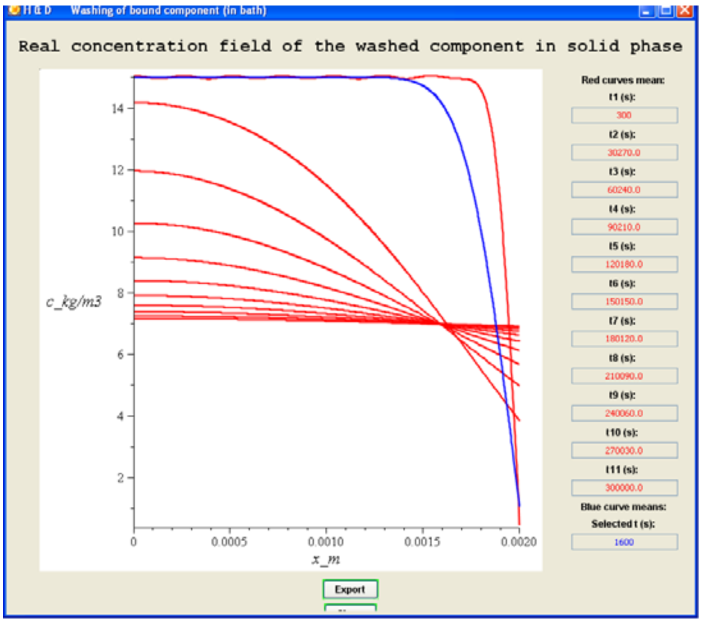

Fig. 9 Window for display of 2D concentration fields in the preselected time

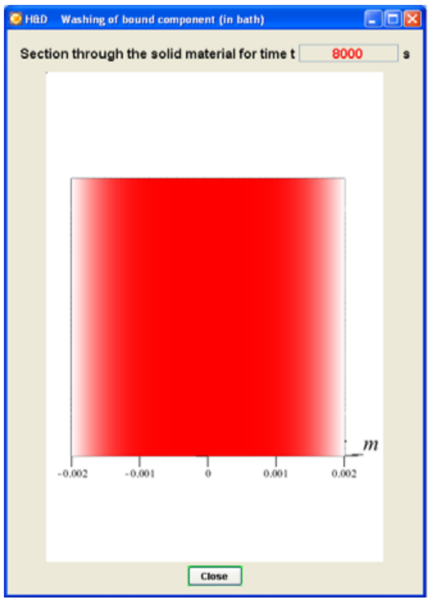

Fig. 10 Window for display of color section through the solid material in required time of washing

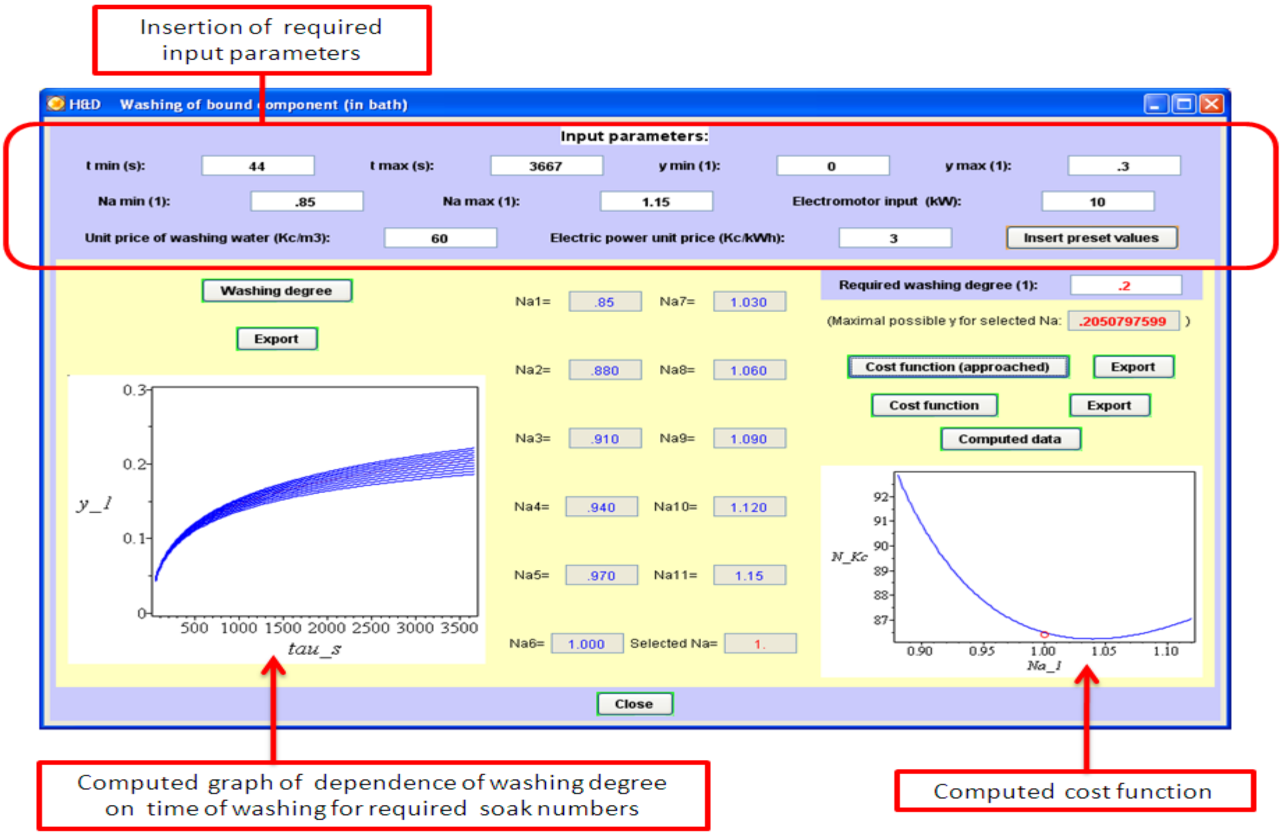

Fig. 11 Window for computing of the cost function

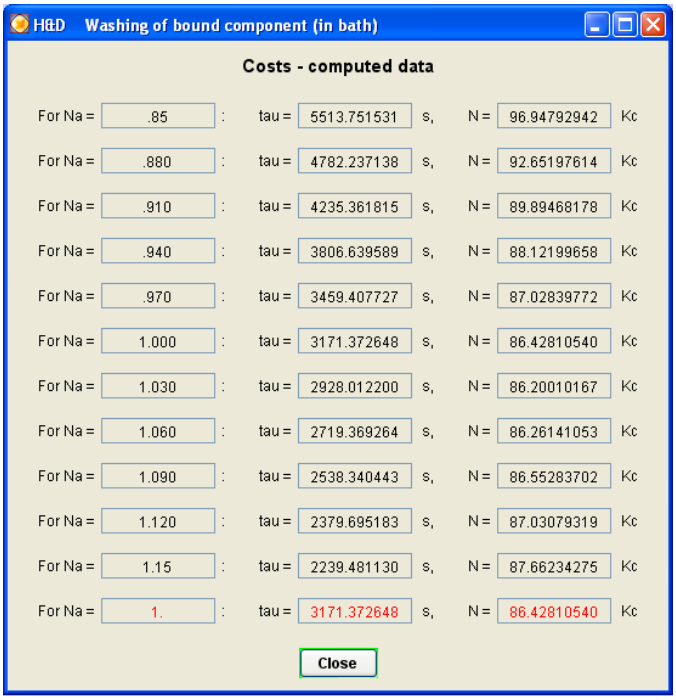

Fig. 12 Window for display of computed data for determination of cost function

V. The Software Application Using

We present our application use 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 $kg \cdot m^{-3}$
Thickness of solid material $2b$:	4 mm
Effective diffusion coefficient D:	$1 \cdot 10^{-8}$ $m^2 \cdot s^{-1}$
Porosity of solid material ε:	0.5
Fixing power A:	5
Input of electromotor to the drive of machinery P:	10kWh
Electric power unit price K_E:	0.5 €$\cdot kW^{-1} \cdot h^{-1}$
Unit price of washing liquid K_V:	2 €$\cdot m^{-3}$
Required washing degree y_0:	0.35

Fig. 13 illustrates course of washing in the solid material under above mentioned conditions. Fig. 14 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.

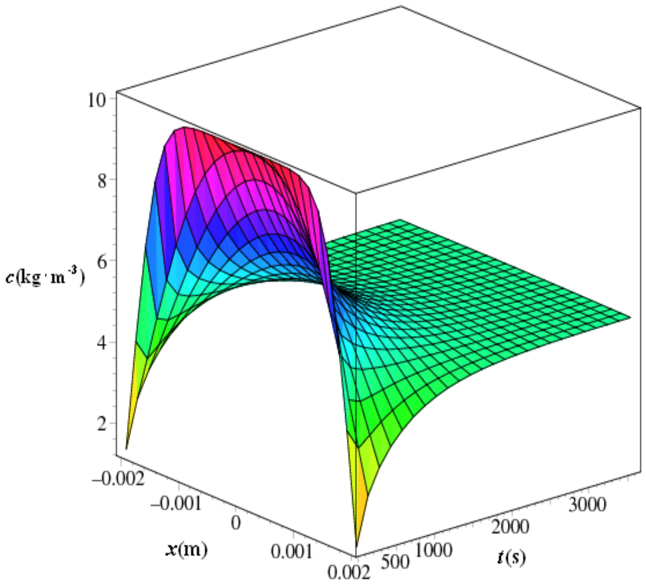

Fig. 13 Bound component concentration field in solid material $c(x, t)$ during washing

As you can see in Fig. 13 and Fig. 14, 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.

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 processes cost.

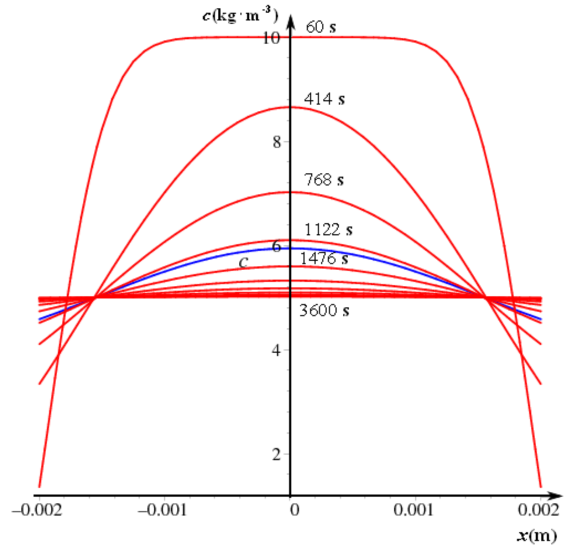

Fig. 14 Concentration field in the solid material in the specific time of washing

In the Fig. 15 we show computed processes costs under the given conditions. The obtained results show that washing process is advantageous under the specified conditions.

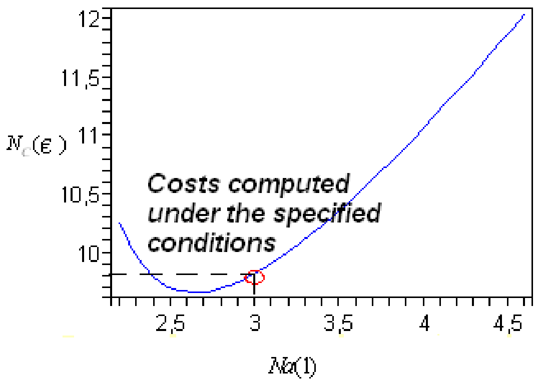

Fig. 15 Computed processes costs

VI. 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 washing liquid 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 succesfully verified by laboratory experiments for deliming process [9]. The main advantage of this work is that the optimal consumption washing liquid to remove of washed component from solid material into the bath. The application will also be used for description and optimization of other processes which are based on the same mechanism as we described in this paper.

VII. LIST OF SYMBOLS

V	volume of solid material	m^3
V_0	volume of washing liquid	m^3
t	time	s
c	volume concentration of washed component in solid material	$kg \cdot m^{-3}$
c_o	volume concentration of washed component in bath	$kg \cdot m^{-3}$
c_p	initial concentration of washed component in solid material	$kg \cdot m^{-3}$
c_A	volume concentration of washed component bound into solid material	$kg \cdot m^{-3}$
D	effective diffusion coefficient	$m^2 \cdot s^{-1}$
D^*	modified diffusion coefficient	$m^2 \cdot s^{-1}$
x	position coordinate	m
b	half thickness of solid material	m
ε	porosity of solid material	1
Na	soak number	1
q_n	n^{-th} root of a certain transcendent equation	1
A	sorption coefficient (fixing power)	1
B	sorption coefficient	$m^3 \cdot kg^{-1}$
S	area of solid material	m^2
F_o	Fourier number	1
C	dimensionless volume concentration of washed component in solid material	1
C_0	dimensionless volume concentration ofwashed component in bath	1
X	dimensionless space coordinate	1
y	washing degree	1
y_0	required washing degree	1
P	input of electromotor to the drive of machinery	kWh
K_E	electric power unit price	$€\cdot kW^{-1}\cdot h^{-1}$
K_V	unit price of washing liquid	$€\cdot m^{-3}$
N_E	electric energy to the drive of machinery costs	€
N_V	washing liquid costs	€
N_C	the main processes costs	€

REFERENCES

[1] D. Janáčová, "Modeling of Extraction Processes", Habilitation work, TBU Zlin, 2003. (in Czech)

[2] K. Kolomazník, D. Janáčová, Z. Prokopová, "Modeling of Raw Hide Soaking", in *WSEAS Transactions on Information Science and Applications*, Hellenic Naval Academy, Ostrava Poruba, 2005.

[3] K. Kolomazník, et al., *Modeling of dynamical systems*, Brno: VUT Brno, 1988. (in Czech)

[4] J. Crank, *The Mathematics of Diffusion*, 2nd Ed. Clarendon Press, Oxford 1977.

[5] D. Janáčová, et al., "Washing Processes Optimization", in *International Union of Leather Technologists and Chemists Societies*, London, 1997.

[6] K. Kolomazník, T. Fürst, D. Janáčová, M. Uhlířová, V. Vašek, "Three Dimensional Transport Model Using in Soaking Process", in *WSEAS Transactions on Computer Research*, WSEAS World Science and Engineering Academy and Science, Queensland, 2007.

[7] K. Kolomazník, D. Janáčová, V. Vašek, M. Uhlířová, "Control algorithms in a minimum of main processing costs for production amaranth hydrolyzates", in *WSEAS Transactions on Information Science and Applications*, WSEAS World Science and Engineering Academy and Science, Athens, 2006.

[8] J. Dolinay, et al., "New Embedded Control System for Enzymatic Hydrolysis", in Proceedings of the 8th WSEAS International Conference on Applied Informatics and Communications, Rhodes, Greece, 2008, p. 174.

[9] H. Charvátová, "Modeling of pelt chemical deliming", Dissertation work, Tomas Bata University in Zlin, Zlin, 2007. (in Czech)

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