Computer Simulation of Bound Component Washing To Minimize Processing Costs

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In this paper we focused on the optimization of the washing processes because many technological processes are characterized by large consumption of water, electrical energy and auxiliary chemicals mainly. For this reason it is very important to deal with them. For the optimization of 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 appropriate for the automatic control of washing process.

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

Introduction

The purpose of the washing process is to wash out the undesirable components from solid phase by water (washing 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.

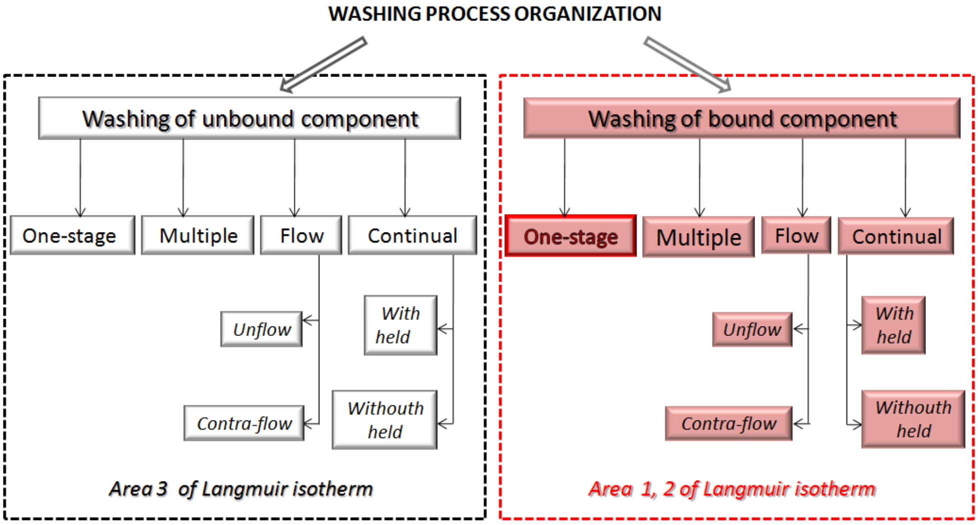

Fig. 1: The cases of washing processes adjustment.

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(Review and revised version 15. 09. 2011)

Theory

For next procedure of the washing process optimizing it is substantial in which part of the sorption isotherm a state of washed component can be found (Fig.2) . In the *Area 3* the washed component is free (does not bind), in the *Area 2* the washed component is bound to solid phase. In this area it is also possible to delimitate *Area 1*, in which the sorption dependence is practically linear. The constant of proportionality (an equilibrium constant of sorption) A characterizes the strength of linkage to solid phase, i.e. largely it can determine how the washing process is effective in this area.

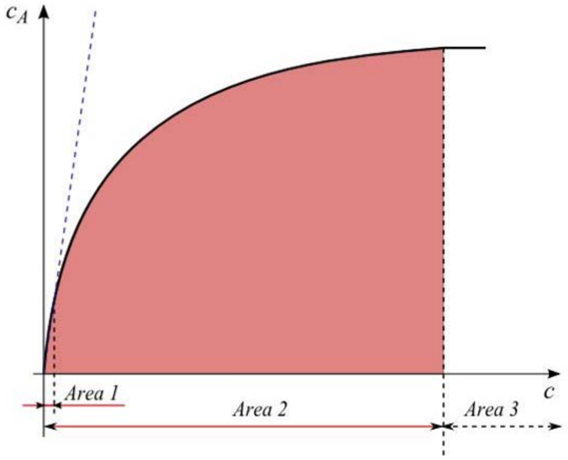


Fig. 2: Langmuir sorption isotherm.

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

The easiest possibility of the sorption constants setting A, B of Langmuir isotherm is directly use of its quantification. 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, the indirect method only incumbent in analyze of liquid phase was designed. To this purpose can be derived dependence

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

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 $B \cdot c$ in equation (1) vanish on 1, it means $1 >> B \cdot c$. Then can be written

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

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

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

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

$$C_o^* = \frac{c_s}{c_o} = \varepsilon(K+1) + Na \tag{5}$$

Mathematical Model of the 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 content of washed up component ions 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 components.

$$\frac{D}{1+A}\cdot\frac{\partial^2 c}{\partial x^2}=\frac{\partial c}{\partial t}+\frac{\partial c_A}{\partial t},\ t>0,\ 0\leq x\leq b \tag{6}$$

$$\frac{\partial c}{\partial x}(b,t)=-\frac{V_o}{D\cdot S}\cdot\frac{dc_o}{dt}(t) \tag{7}$$

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

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

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

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

where sorption constants A and B are determined from Langmuir isotherm (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 equation of Langmuir sorption isotherm (1). Condition (7) shows the initial distribution of washed component concentration in solid phase-material. Equation (8) describes that we use pure water for material bath washing. equation (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 (6) with additional conditions (7)-(11)

$$C=\frac{c}{c_p},\ C_o=\frac{c_o}{c_p},\ F_o=\frac{D\cdot t}{b^2(1+A)},\ X=\frac{x}{b},\ Na=\frac{V_o}{V} \tag{12}$$

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

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

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

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

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 for required washing degree y . Washing degree, which characterizes efficiency of the process, is given by is ratio of mass of washed component to initial mass of washed component in the solid material

$$y=\frac{Na}{\varepsilon(1+A)+Na}-2\frac{Na^2}{\varepsilon(1+A)}\sum_{n=1}^{\infty}\frac{\exp(-F_oq_n^2)}{\varepsilon(1+A)+\frac{q_n^2Na^2}{\varepsilon(1+A)}+Na} \tag{15}$$

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

$$N_C=N_V+N_E \tag{16}$$

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

$$N_E = K_E \cdot P \cdot t \tag{17}$$

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_o

$$N_V = K_V \cdot V_o \tag{18}$$

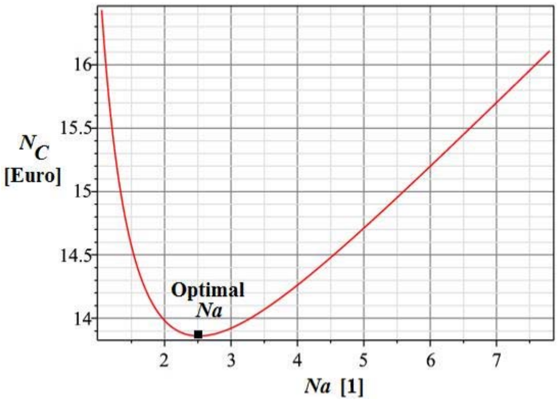


Fig. 3: The cost function.

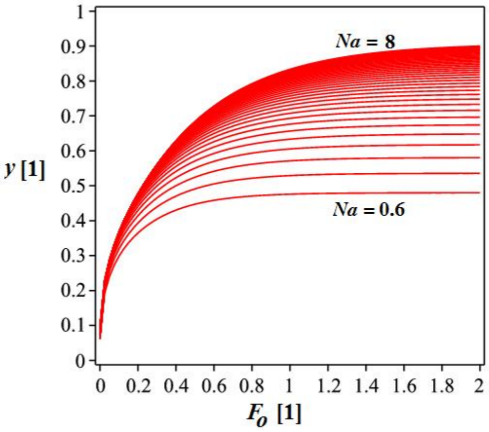


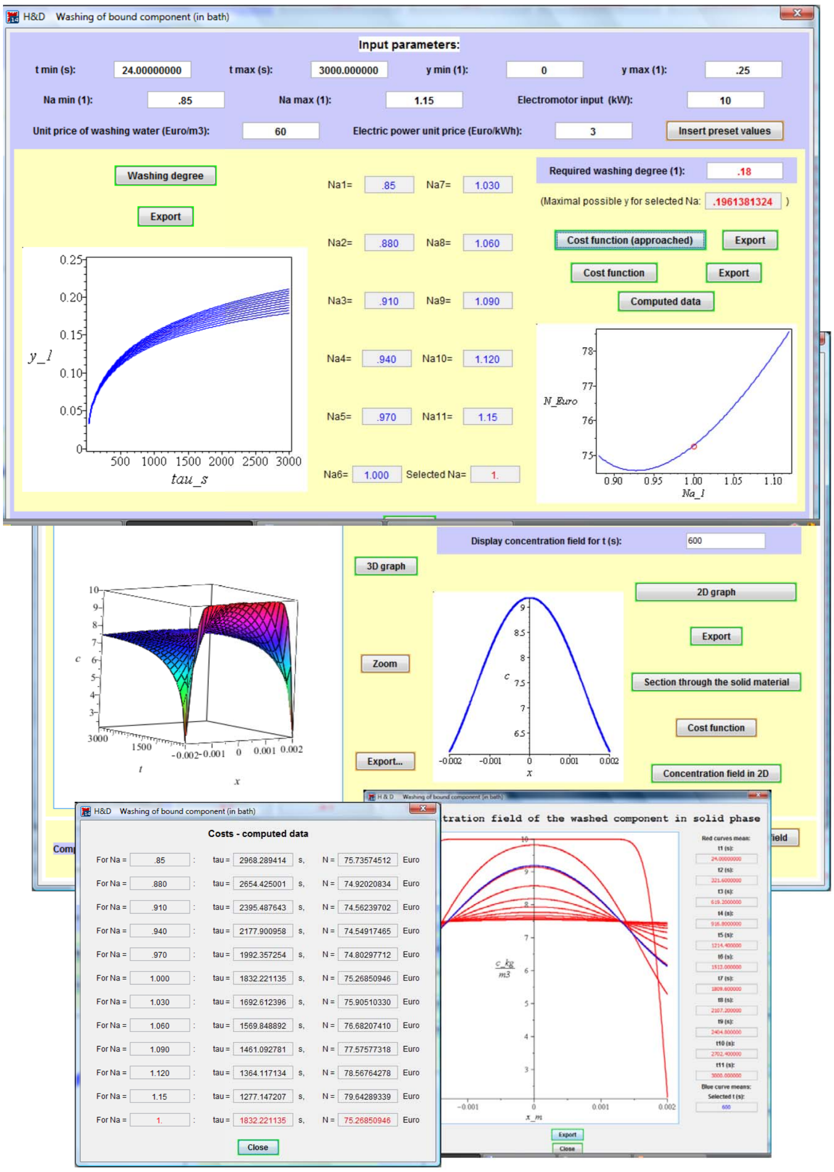
Fig. 4: Dependence of the washing degree on the dimensionless time.

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. Example of the cost function you can see in Fig. 3.

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, on the dimensionless time F_o and that for the corresponding soaking number Na (Fig. 4).

For computation of the dependence of washing degree on the dimensionless time (Fig.4) and cost function (Fig.3) we used these parameters:

$$b = 2.5\text{ mm},\ D = 1.10^{-9}\mathtt{m}^2.\mathtt{s}^{-1},\ \varepsilon = 0.5,\ A = 0.3,\ c_p = 10\mathtt{kg.m}^{-3},\ y_o = 0.43,\ P = 15\text{ kW},\ K_V = 0.5\mathtt{Euro.m}^{-3},$$
$$K_E = 2\mathtt{Euro.kW}^{-1}.\mathtt{h}^{-1}.$$



t min (s): 24.00000000 t max (s): 3000.000000 y min (1): 0 y max (1): .25

Na min (1): .85 Na max (1): 1.15 Electromotor input (kW): 10

Unit price of washing water (Euro/m3): 60 Electric power unit price (Euro/kWh): 3

Required washing degree (1): .18

(Maximal possible y for selected Na: .1961381324)

Na1= .85 Na7= 1.030
Na2= .880 Na8= 1.060
Na3= .910 Na9= 1.090
Na4= .940 Na10= 1.120
Na5= .970 Na11= 1.15
Na6= 1.000 Selected Na= 1.

Display concentration field for t (s): 600

Red curves mean:
t1 (s): 24.00000000
t2 (s): 321.6000000
t3 (s): 619.2000000
t4 (s): 916.8000000
t5 (s): 1214.400000
t6 (s): 1512.000000
t7 (s): 1809.600000
t8 (s): 2107.200000
t9 (s): 2404.800000
t10 (s): 2702.400000
t11 (s): 3000.000000
Blue curve means:
Selected t (s): 600

Costs - computed data

For Na = .85 : tau = 2968.289414 s, N = 75.73574512 Euro
For Na = .880 : tau = 2654.425001 s, N = 74.92020834 Euro
For Na = .910 : tau = 2395.487643 s, N = 74.56239702 Euro
For Na = .940 : tau = 2177.900958 s, N = 74.54917465 Euro
For Na = .970 : tau = 1992.357254 s, N = 74.80297712 Euro
For Na = 1.000 : tau = 1832.221135 s, N = 75.26850946 Euro
For Na = 1.030 : tau = 1692.612396 s, N = 75.90510330 Euro
For Na = 1.060 : tau = 1569.848892 s, N = 76.68207410 Euro
For Na = 1.090 : tau = 1461.092781 s, N = 77.57577318 Euro
For Na = 1.120 : tau = 1364.117134 s, N = 78.56764278 Euro
For Na = 1.15 : tau = 1277.147207 s, N = 79.64289339 Euro
For Na = 1. : tau = 1832.221135 s, N = 75.26850946 Euro

Fig. 5: Show of user interface of the software application.

Simulation of the 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 Maple 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 qn are obtained by numeric solution of equation (14). After this calculation, the dimensionless concentration field $C(X,F_o)$ or concentration field $c(x,t)$.The concentration field can be visualized as a surface $c(x,t)$ $(C(X,F_o))$ (3D graphics) or as a curve $c(x)$ $(C(X))$ (2D graphics) for specific dimensionless time F_o. The other window can compute dependence of the washing degree on time and the cost curve which we described in the previous section.

Example of the Washing Process Computer Simulation

We present our application using in the following example which describes bound component removing that proceeds under these conditions:
Volume of washing liquid V: 3 $\mathtt{m}^3$
Volume of solid material in bath V_o: 1 $\mathtt{m}^3$
Initial concentration of bound component in material c_p: 6 $\mathtt{kg.m}^{-3}$
Thickness of solid material $2b$: 4 mm
Effective diffusion coefficient D: 1.10^{-8} $\mathtt{m}^2\mathtt{s}^{-1}$
Porosity of solid material ε: 0.5
Sorption constant A: 3
Required washing degree y_0: 0.25
Input of electromotor to the drive of machinery P: 10 $\mathtt{kWh}$
Electric power unit price K_E: 2.5 $\mathtt{Euro.kW}^{-1}\mathtt{.h}^{-1}$
Electric power unit price K_V: 0.2 $\mathtt{Euro.m}^{-3}$

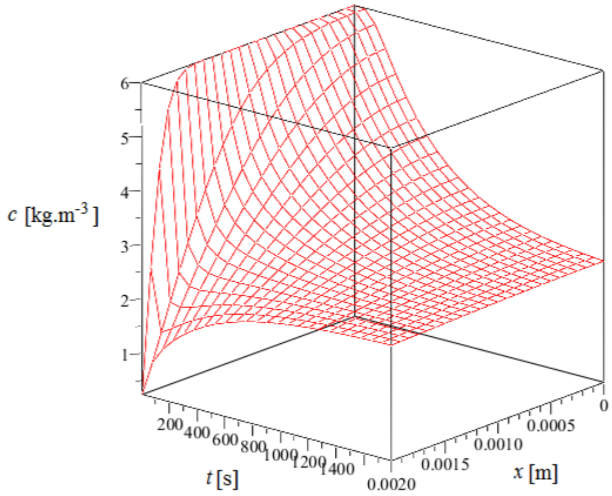


Fig. 6: Bound component concentration field in solid material during washing.

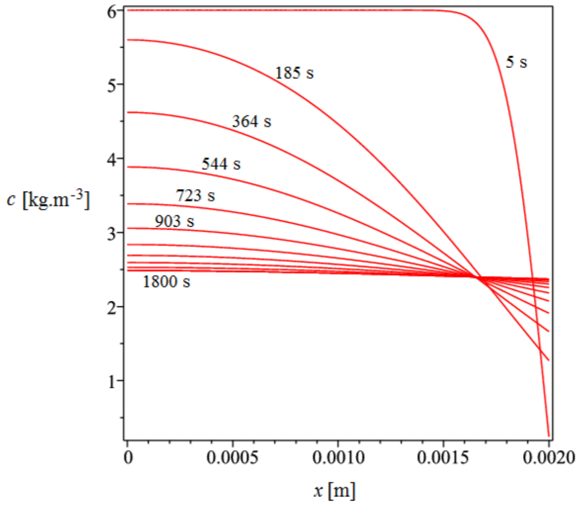


Fig. 7: Concentration field in the solid material in the specific operation time.

Fig. 6 illustrates course of washing in the solid material under above mentioned conditions. Fig. 7 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. 6 and Fig. 7 in the time between approximately 1000 and 1800 seconds, the bound component concentration decreases nearly negligible because most of bound component already diffused from the material into the washing bath. 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. In the Fig. 8 we show determination of the operating time to achieve required washing degree 0.25 in detail. In the studied case the time is about 950 seconds.

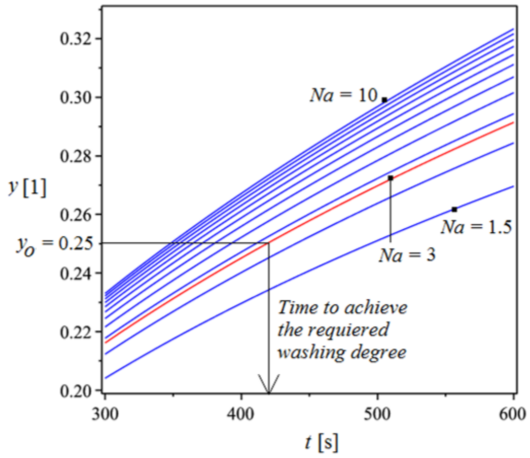


Fig. 8: Determination of the operating time to achieve requiered washing degree in detail.

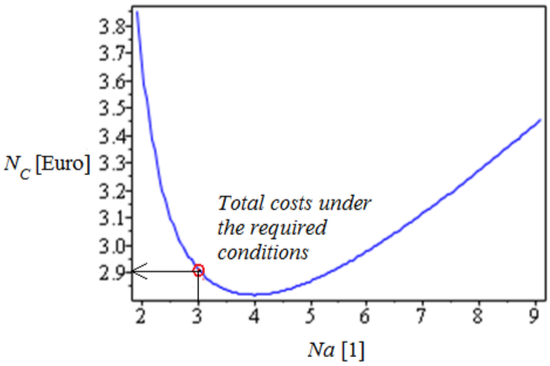


Fig. 9: Computed cost function.

Finally, we computed the cost function. As you can see in Fig. 9, the total costs are about 2.5 Euro. The optimal soaking number *Na* is approximately 3.75 - 4.25 under the studied conditions.

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 deliming process course, as a case of the washing process, was also verified by laboratory experiments [3]. The main advantage of this work is that the optimal consumption of water, chemical agents and energy determine effective course of arbitrary bound component extraction from solid phase in bath system. The application will also be used for description and optimization of other washing (extraction) processes during natural polymers treatment.

Acknowledgement

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic under the Research Plan No. MSM 7088352102 and by the European Regional Development Fund under the project CEBIA-Tech No. CZ.1.05/2.1.00/03.0089.

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List of Symbols

Tab. 1: List of symbols.

Symbol	Meaning	Unit
V	Volume of solid phase (material)	$\mathtt{m}^3$
V_o	Volume of washing water	$\mathtt{m}^3$
Na	Soaking number(dimensionless consumption of washing liquid)	1
t	Time	s
c	Concentration of component in material	$\mathtt{kg.m}^{-3}$
c_A	Concentration of bound component in material	$\mathtt{kg.m}^{-3}$
c_o	Concentration of component in bath	$\mathtt{kg.m}^{-3}$
c_p	Initial concentration of component in material	$\mathtt{kg.m}^{-3}$
D	Effective diffusion coefficient of washing component in material	$\mathtt{m}^2.\mathtt{s}^{-1}$
x	Position coordinate	m
b	Half thickness of material	m
ε	Porosity (ratio of poroses volume to total material volume)	1
q_n	n-th root of a certain transcendent equation	1
A	Equilibrium sorption constant	1
B	Sorption constant	$\mathtt{m}^3.\mathtt{kg}^{-1}$
S	Area of material	$\mathtt{m}^2$
F_o	Fourier number (dimensionless time)	1
C	Dimensionless concentration of component in material	1
C_o	Dimensionless concentration of component in bath	1
X	Dimensionless space coordinate	1
y	Washing degree	1
y_o	Required washing degree	1
P	Input of electromotor to the drive of machinery	kWh
K_E	Electric power unit price	$\mathtt{Euro.kW}^{-1}.\mathtt{h}^{-1}$
K_V	Unit price of washing liquid	$\mathtt{Euro.m}^{-3}$
N_E	Electric energy to the drive of machinery costs	Euro
N_V	Washing liquid costs	Euro
N_C	The main processes costs	Euro