

The Mathematical Modeling of Bound Component Extraction

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Abstract—The paper deals with application of mathematical modeling in process engineering. Our contribution contains mathematical deterministic models of extraction processes which are part of technology processes very often. We suggested them for their optimization. Without mathematical simulation and optimization are extraction processes of bound component connected with enormous consumption of extraction liquid.

Keywords—Mathematical modeling, extraction, diffusion process.

I. INTRODUCTION

WE worked out mathematic models describing extraction of bound component from material because is often solved problem of this in extraction technology processes. On the base of them, we suggested goal cost functions for optimization of extraction processes [3], [4]. The main part of operating costs connected with the consumption of active aqueous solutions, eventually technological extraction liquid bath, depends on the operating time, which simultaneously determines the consumption of electrical energy necessary to the drum drive (move). The bigger liquid consumption, the bigger gradient of diffusive components concentration and the bigger decrease of operating time needed for the achievement of required level of the material [1]. The result of mentioned

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consideration is the minimum main part of operating costs in their dependence on the liquid consumption. Our task is to estimate this minimum and to compare the result with real process [9].

II. THE GOAL COST FUNCTION

It is possible to find the optimum of consumption of liquid 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 by liquid we assumed that we are able to eliminate component from the material by the liquid and that the main operating costs N_T of considered process are given by the sum of the consumed electric energy to the drive of machinery costs N_E and the consumed extraction liquid costs N_L . The following physico-chemical model serves for the determination of minimum operating costs [3]:

$$N_T = N_L + N_E = K_L V_0 + K_E P t . \quad (1)$$

III. EXTRACTION PROCESSES

It is possible to divide the extraction processes of bound component into several cases according to the way of adjustment:

One-stage extraction

The balance of extracted component we can write [3], [6], [7]:

$$c_p V + c_{Ap} V = V_0 c_0 + cV + c_A V . \quad (2)$$

In equilibrium

$$\varepsilon \cdot C_0 = C . \quad (3)$$

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 extraction process is

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

$$c_A = \frac{Kc}{Bc + 1} \quad (4)$$

For very low concentrations, when $Bc \ll 1$, it is possible to delimitate the area of linear dependence of sorption isotherm by relation:

$$c_A = K \cdot c \quad (5)$$

For high concentrations, when $Bc \gg 1$, it is approximately

$$c_A = K / B, \quad (6)$$

which is the maximum value of absorbed component concentration, sometimes called the sorption capacity of solid phase.

After modification of equation (2) we obtain:

$$c_0 = \frac{c_p(1+K)V}{V_0 + \varepsilon(1+K)V} = \frac{c_p(1+K)}{Na + \varepsilon(1+K)} \quad (7)$$

Total degree of extraction is represented next equation

$$y = \frac{c_0 V_0}{V(c_p + Kc_p)} = \frac{c_0 Na}{c_p(1+K)}, \quad (8)$$

where $Na = \frac{V_0}{V}$ and means dimensionless consumption of liquid.

For next modification c_0 we can use previous equation (8):

$$y = \frac{Na}{Na + \varepsilon(1+K)} \quad (9)$$

Fig. 1 shows the influence of degree of extraction on fixing power constant K .

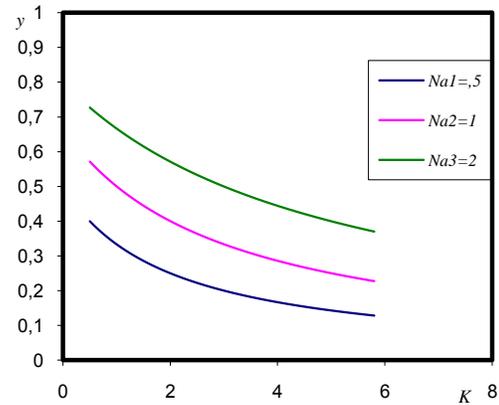


Fig. 1 Influence of degree of extraction on fixing power constant K

A. One-stage extraction - diffusion model

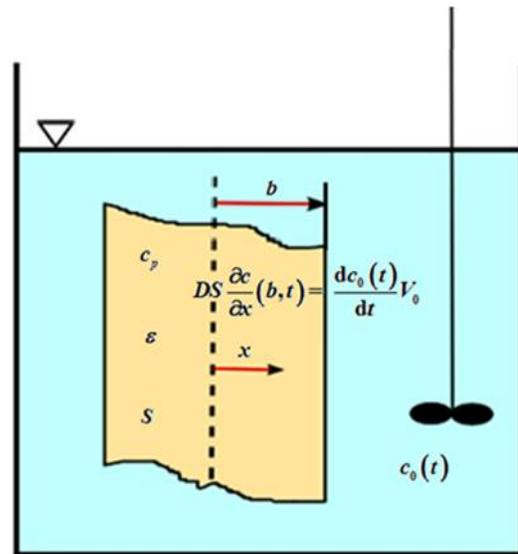


Fig. 2 Model of one-stage extraction process

In this process, the material is put into the extraction liquid. The extraction liquid flows neither in nor out of the bath.

Under assumptions that bound component content in material is lower than its solubility in the same volume of extraction 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 extraction of material sample by diffusion model of transport of extract out component [8], [9].

$$\frac{D}{K+1} \cdot \frac{\partial^2 c(x,t)}{\partial x^2} = \frac{\partial c(x,t)}{\partial t}, \quad t > 0, 0 \leq x \leq b \quad (10)$$

$$\frac{\partial c}{\partial x}(b,t) = - \frac{V_0}{D \cdot S} \cdot \frac{dc_0(t)}{dt} \quad (11)$$

$$c(x,0) = c_p \tag{12}$$

$$c_0(0) = 0 \tag{13}$$

$$\frac{\partial c}{\partial x}(0,t) = 0 \tag{14}$$

$$c(b,t) = \varepsilon \cdot c_0(t). \tag{15}$$

Equation (10) represents component ions diffusion from material in the direction of extraction liquid bath. The expression of the right hand side last term of equation depends on desorption mechanism of extraction 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 bound component c by the relation of Langmuir's sorption isotherm [3]. Condition (12) shows the initial distribution of component concentration in solid phase-material. Relation (13) describes that we use pure water for material bath extraction. Relation (9) holds under condition of a perfectly mixed liquid phase. Boundary condition (14) 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.

Dimensionless variables for the solution of equation (10) with additional conditions (11-15) are:

$$C = \frac{c}{c_p}, C_0 = \frac{c_0}{c_p}, Fo_o = \frac{Dt}{b^2(1+K)}, X = \frac{x}{b} \tag{16}$$

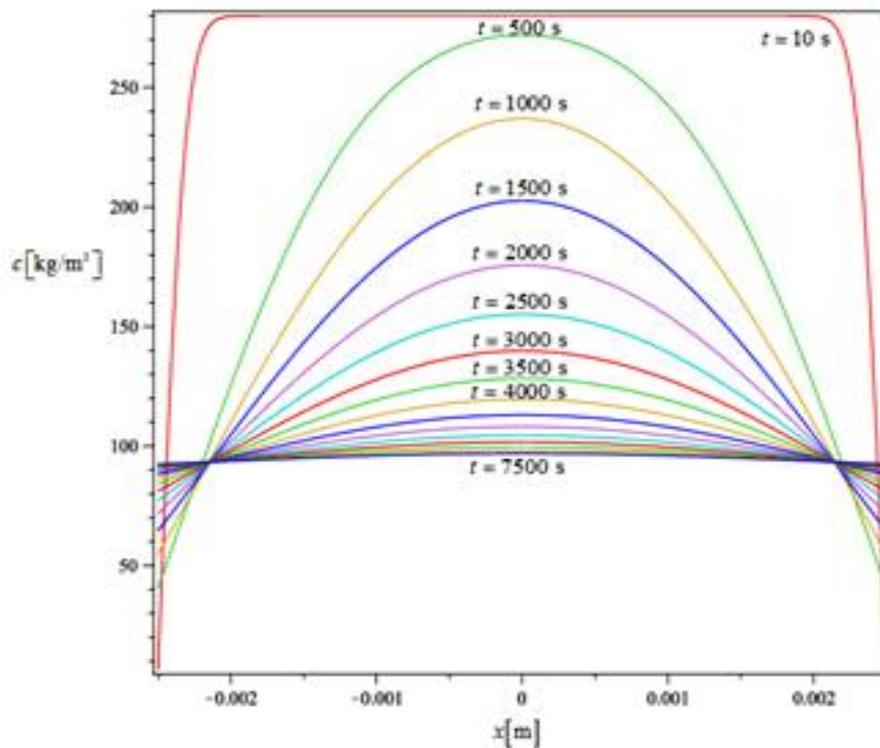


Fig. 3 Concentration field of extraction component in the material during process

$$b = 0.0015 \text{ m}; D = 2 \cdot 10^{-8} \text{ m}^2 \text{ s}^{-1}; V = 1 \text{ m}^3; \varepsilon = 0.5.$$

By means of Laplace transformation we obtain analytic solution. Final solution of extraction degree for this case is:

$$y = \frac{C_0 Na}{1+K} - \frac{Na}{\varepsilon(1+K)+Na} - 2 \frac{Na^2}{\varepsilon(1+K)} \sum_{n=1}^{\infty} \frac{\exp(-F_0 q_n^2)}{\varepsilon(1+K) + \frac{q_n^2 Na^2}{\varepsilon(1+K)} + Na} \tag{17}$$

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

$$-\frac{Na \cdot q}{\varepsilon \cdot (1+K)} = \tan(q). \tag{18}$$

In the Fig. 4 we show detailed sketch of determination time to reaching demanded extraction degree

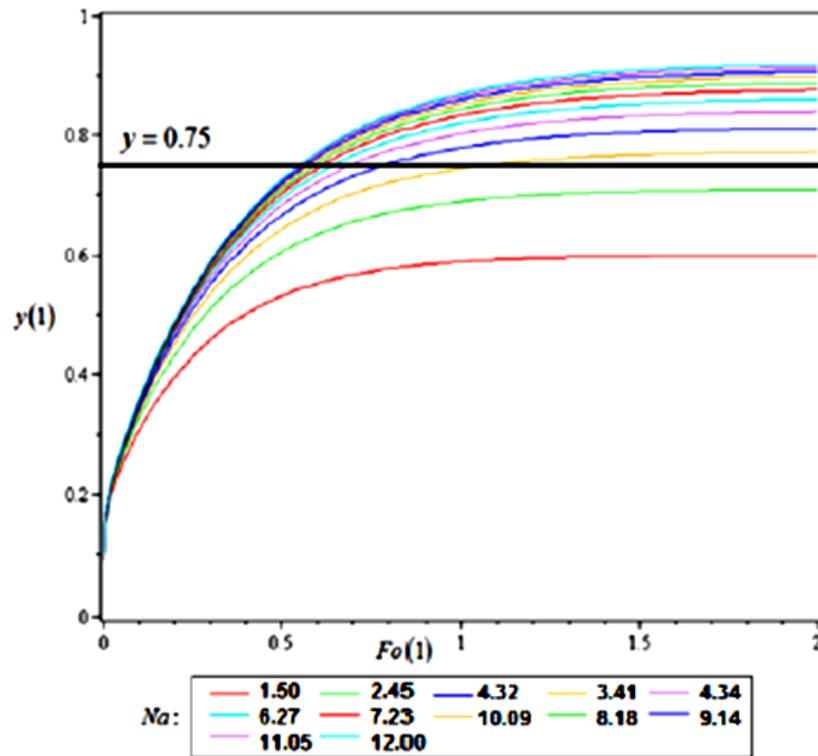


Fig. 4 Detail of determination time to reaching demanded extraction degree

$b = 0.0015 \text{ m}; D = 2 \cdot 10^{-8} \text{ m}^2\text{s}^{-1}; V = 1 \text{ m}^3; \varepsilon = 0.5, y = 0.75.$

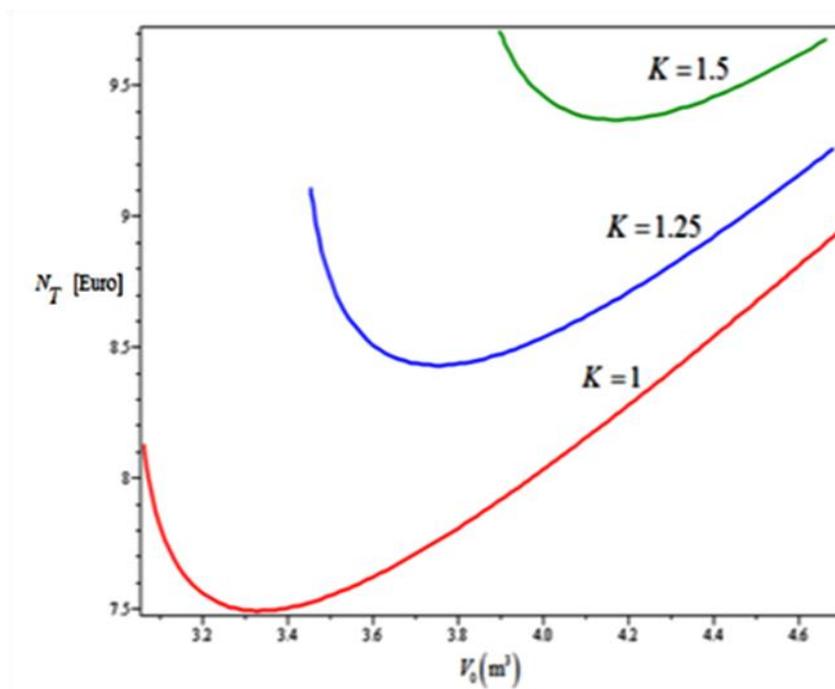


Fig. 5 Cost functions - determination of the optimal extraction number for variable K

$b = 0.0015 \text{ m}; D = 2 \cdot 10^{-8} \text{ m}^2\text{s}^{-1}; V = 1 \text{ m}^3; \varepsilon = 0.5, y = 0.75;$
 $N_E = 0.3 \text{ Euro} \cdot \text{W}^{-1}\text{h}^{-1}; N_V = 1.6 \text{ Euro} \cdot \text{m}^{-3}; P = 10 \text{ kW}.$

B. Flow continual extraction - diffusion model

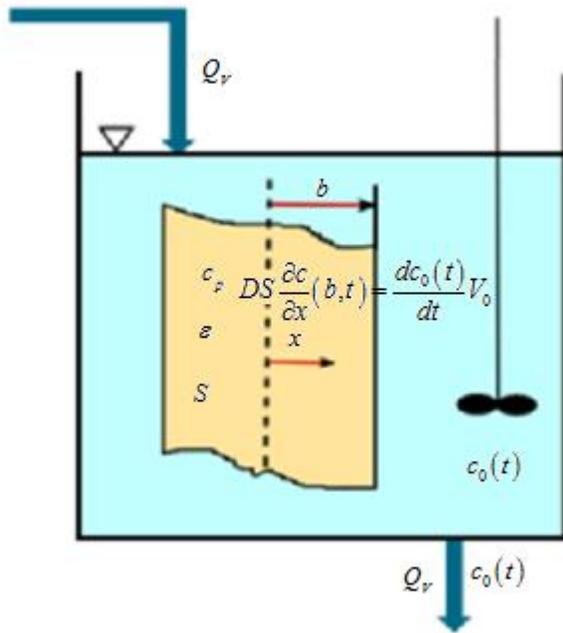


Fig. 6 Model of flow extraction process

By washing in the low system, water is continuously brought to rotating equipment. This process can be described by equations (19 - 24) [3].

$$\frac{D}{1+K} \frac{\partial^2 c}{\partial x^2}(x,t) = \frac{\partial c}{\partial \tau}(x,t) \quad , 0 < t, \quad 0 \leq x \leq b \quad (19)$$

$$C(X, F_0) = 2 \sum_{n=1}^{\infty} \frac{[DV_0 q_n^2 - (1+K)Q_v b^2] e^{-q_n^2 F_0} \cos(q_n \cdot X)}{q_n [DV_0 q_n (q_n \sin q_n - 2 \cos q_n) - (1+K)(DV \varepsilon + Q_v b^2) \sin q_n - (1+K)DV \varepsilon q_n \cos q_n]} \quad (27)$$

The roots q_n can be calculated from the transcendent equation

$$\tan q = \frac{(1+K)Q_v b^2 - q^2 V_0 D}{(1+K)DV \varepsilon q} \quad (28)$$

$$y = 1 + 2 \sum_{n=1}^{\infty} \frac{[DV_0 q_n^2 - (1+K)Q_v b^2] e^{-q_n^2 F_0} \cos(q_n)}{q_n^3 + \frac{2q_n^3 \varepsilon (1+K)}{Na_0 (q_n^2 - L)} - \frac{q_n \varepsilon (1+K)}{Na_0} + \frac{q_n^3 \varepsilon^2 (1+K)^2}{Na_0^2 (q_n^2 - L)} - Lq_n} \quad (29)$$

$$\frac{\partial c}{\partial x}(0,t) = 0 \quad (20)$$

$$c_0(0) = 0 \quad (21)$$

$$c(x, 0) = c_p \quad (22)$$

$$c(b,t) = \varepsilon \cdot c_0(t) \quad (23)$$

$$- \frac{D}{1+K} S \frac{\partial c}{\partial x}(b,t) = Q_v c_0(t) + V_0 \cdot \frac{dc_0}{dt}(t) \quad (24)$$

where the dimensionless quantities have the form:

$$L = \frac{Q_v b^2 (1+K)}{V_0 D} \quad (25)$$

$$Na_0 = \frac{V_0}{V} \quad (26)$$

By comparing of the above mentioned methods, in the flow system, the increase in the water level is compensated by the outflow of waste water. The advantage of this equation lies in the permanent contact of hide with water, which accelerates the extraction process. A disadvantage is high water consumption. Decantation washing y is very time-consuming, but on the other hand requires much less plain water than it is in flow system.

By Laplace transformation we obtain analytical solution describing concentration field in solid phase (27):

The extraction degree can be calculated according to equation (29):

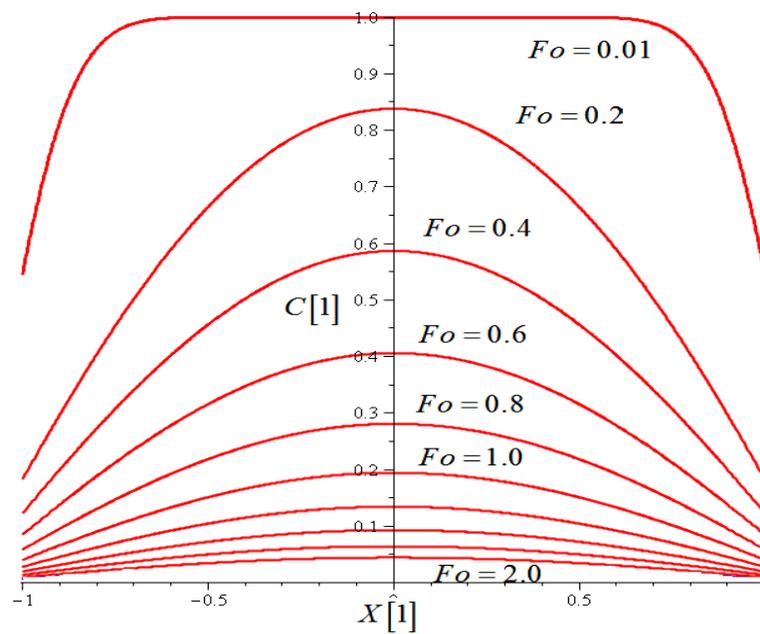


Fig. 7 Concentration fields field of extraction component in the material in the flow system

$$b = 0.0015 \text{ m}; D = 2 \cdot 10^{-8} \text{ m}^2 \text{ s}^{-1}; \varepsilon = 0.5; Q_V = 8 \cdot 10^{-4} \text{ m}^3 \text{ s}^{-1}; K = 1.$$

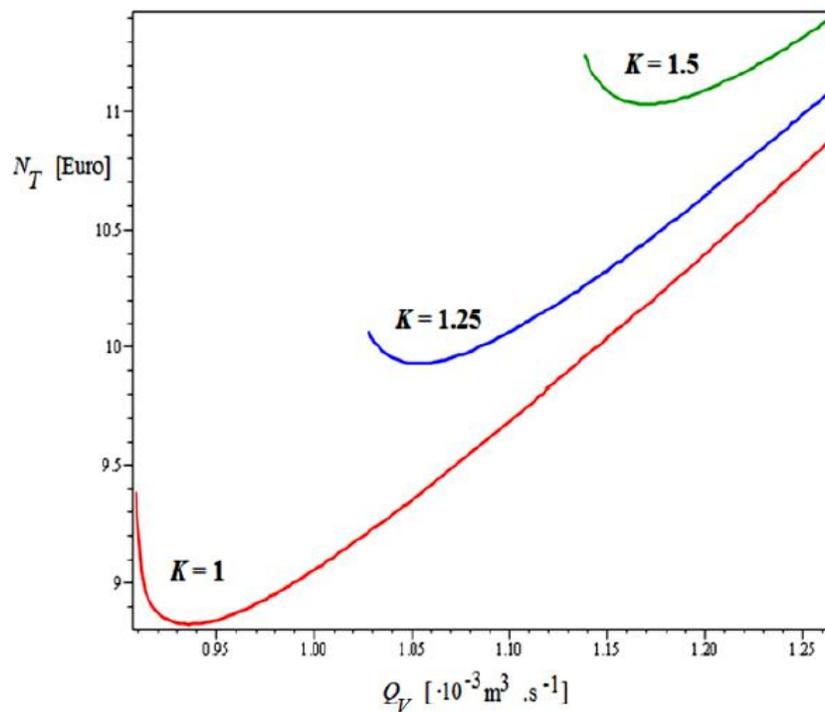


Fig. 8 Cost functions by continual extraction - determination of the optimal extraction number for variable K

$$b = 0.0015 \text{ m}; D = 2 \cdot 10^{-8} \text{ m}^2 \text{ s}^{-1}; \varepsilon = 0.5; y = 0.75; N_E = 0.3 \text{ Euro} \cdot \text{W}^{-1} \text{ h}^{-1}; N_V = 1.6 \text{ Euro} \cdot \text{m}^{-3}; P = 10 \text{ kW}.$$

IV. CONCLUSION

The target function is dependent on the mathematical model of the real process and on the main purpose to be achieved by this operation. For the design of the control of extraction we have chosen minimisation of operating costs. The volume of extraction and the time of operation should be chosen so as to minimize the costs of water and power necessary for drum. We can obtain the same quality of extraction by using a lower volume of water and prolonged extraction time. At the beginning the cost function, total extraction time is decreasing, because for short extraction times the water volume required is increasing of proportion and for longer times it is increasing because reduced water consumption cannot compensate the long operation time connected with power consumption. Quantitative description for mentioned cases of extraction processes were verified and implemented. We created the program for calculation of the extraction process is to extract out the undesirable components from solid phase by solvent in which the extracted component is not very well soluble during extraction process.

V. LIST OF SYMBOLS

b - half thickness of the material, [m];
 B - sorption constant, [$\text{m}^3 \cdot \text{kg}^{-1}$];
 c - concentration of component in the material, [$\text{kg} \cdot \text{m}^{-3}$];
 c_A - concentration of extracted bound component in the material, [$\text{kg} \cdot \text{m}^{-3}$];
 c_0 - concentration of component in the liquid phase, [$\text{kg} \cdot \text{m}^{-3}$];
 c_{Ap} - initial concentration of extracted bound component in the material, [$\text{kg} \cdot \text{m}^{-3}$];
 cp - initial concentration of extracted component in the material, [$\text{kg} \cdot \text{m}^{-3}$];
 C - dimensionless concentration of component in the material, [1];
 C_0 - dimensionless concentration of component in the liquid phase, [1];
 D - diffusion coefficient, [$\text{m}^2 \cdot \text{s}^{-1}$];
 Fo - Fourier number - dimensionless time, [1];
 K - power of fixing component, [1];
 K_L - price of liquid, [$\text{Euro} \cdot \text{m}^{-3}$];
 K_E - price of electric energy, [$\text{Euro} \cdot \text{W}^{-1} \cdot \text{h}^{-1}$];
 L - dimensionless volume rate of flow, [1];
 Na, Na_0 - dimensionless volume of liquid bath, [1];
 N_T - total main operating costs, [Euro];
 N_L - extraction liquid costs, [Euro];
 N_E - electric energy costs, [Euro];
 P - power of engine, [W];
 V - volume of the material, [m^3];
 V_0 - volume of the liquid phase, [m^3];
 x - space coordinate, [m];
 X - dimensionless space coordinate, [1];
 q_n - n^{th} roots of transcendent equation, [1];
 Q_V - volume rate of flow, [$\text{m}^3 \cdot \text{s}^{-1}$];
 S - surface of the material, [m^2];
 t - time, [s];
 y - degree of extraction process, [1];
 ε - porosity of the material, [1].

REFERENCES

- [1] P. Mokrejš, F. Langmaier and M. Mládek, "Acid treatment of Chromed Material Waste from Footwear and Garment Production", *Indian Chemical Engineer*, vol. 4, 2003.
- [2] P. Chalupa, M. Beneš, J. Novák, M. Bařinová, "Control system for chemical thermal processes". In *Latest Trends on Systems - Volume II* - Proceedings of the 18th International Conference on Systems, Santorini, 2014.
- [3] D. Janáčová, et al., "Washing Processes Optimization", *Proceedings of International Union of Material Technologists and Chemists Societies*, London, 1997.
- [4] K. Kolomazník, D. Janáčová, V. Vašek, M. Uhlřivá, "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.
- [5] J. Crank, *The Mathematics of Diffusion*, London: Oxford University Press, 1956.
- [6] H. Charvátová, *Modeling of Pelt Chemical Delimiting*, (Dissertation work) Zlín: Tomas Bata University in Zlín, 2007.
- [7] D. Janáčová D, H. Charvátová, K. Kolomazník K., and V. Vašek, *Creating software applications for solving diffusion problems in the MAPLE interface* (in Czech), Zlín, Tomas Bata University in Zlín, 2012.
- [8] K. Kolomazník, et al. "Modeling of Raw Hide Soaking", in *WSEAS Transactions on Information Science and Applications*, Ostrava Poruba, 2005.
- [9] K. Kolomazník, D. Bailey, M. M. Taylor, "Delimiting of un-bonded and bonded lime from white hide", *Journal of American Leather Chemists Association*, vol. 102, 2007.
- [10] D. Janáčová, V. Vašek, K. Kolomazník, "The cost function for extraction of bound component from material", in *Latest Trends on Systems*. Volume II. Rhodes: Europment, 2014, p. 395-398.
- [11] R. Drga, "Inaccuracy in measuring the IR radiation source temperature thermal camera", (in Czech), in *Automatizacia a riadenie v teorii a praxi*, Košice, Slovak Republic, 2012.
- [12] M. Mañas, M. Staněk, S. Šanda and D. Mañas, "Rychlá příprava prototypů, a reverzní inženýrství v konstrukci dílů a nástrojů", (in Czech) in *Proceedings of the 7th International Tools Conference ITC 2009*, Zlín, 2009.

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