Mathematical modeling of the extraction process of coniferous plants

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Abstract. The article presents the results of a mathematical description of heat and mass transfer processes occurring throughout the volume of the extracted substance. A mathematical model has been developed that describes the regularities of the transition of a solute from a solid to a liquid phase. The procedure of computerized calculation of the extraction process was performed. The dynamics of the relationship between heat and mass transfer processes in the product was studied using the Matlab software package.

1. Introduction

The main process in obtaining target components from plant raw materials of needles is extraction [1,2]. The rate of extraction of target, biologically active substances from conifers by the extraction method is determined by various parameters that complicate generalization and analysis. The extracted component can be in a liquid or solid state, a solid material can be an inert carrier of the target component or interact with it, hold it due to adsorption and other forces. The structure of the solid and the equilibrium conditions affect the extraction process. The theoretical foundations of the extraction process for conifers have not been studied enough. There is no complex model of the process and installation that takes into account the properties of the material and the laws of interaction between two bodies. It is known that the extraction process is the transfer of a substance from one phase to another [3,4].

In a number of studies, the extraction process has been analyzed empirically and experimentally, in which heat and mass transfer are considered separately, and external influences are not taken into account. Therefore, on the basis of mathematical modeling, solve a complex problem, taking into account all the acting factors. Thus, the main tasks are:

- ensuring the uniformity of the distribution of the elements of the dispersed phase in the continuous phase
- study of the movement of solid particles and liquids in the proposed installation;
- study of influencing factors such as the size of a solid particle, the average residence time of particles of a solid phase in the installation.
2. Theoretical basis

Improvement of the organization of the process of extraction of plant materials is achieved due to the design parameters of the apparatus. The process is controlled by changing the technological parameters. The complete mathematical model of the process of extracting biologically active substances from coniferous plants in a discrete-countercurrent installation of an apparatus flowing on a scale includes mathematical models of the processes occurring in the functional closed structural elements of the apparatus.

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The hydrodynamic structure of flows in the liquid phase in such apparatuses can be fixed in the form of an ideal mixing model, according to which the concentration of the extracted component in the solid phase \( a_T \) is described by differential equations of the first order.

In this case, the mathematical description of the change in the concentration of the extracted component in the solid phase is expressed in the following form:

\[
\frac{da_s}{d\tau} = \frac{1}{\tau_{ave}} \left[ a_s^{in} - a_s^{out} \right],
\]

where \( \tau_{ave} \) - average residence time of solid phase particles in the installation; \( a_s^{in}, a_s^{out} \) - respectively, the concentration of the extracted component in the solid phase at the inlet and outlet.

The average residence time of particles can be determined by the formula:

\[
\tau_{ave} = \frac{m_s}{G_s + G_j},
\]

where \( m_s \) - the amount of suspension in the installation.

In turn, \( m_s \) is expressed as:

\[
m_s = \frac{V_s \rho_s}{G_s + G_j},
\]

where \( V_s \) - the volume of the suspension in the installation; \( \rho_s \) - suspension density.

Then expression (2) will take the form:

\[
\tau_{ave} = \frac{V_s \rho_s}{G_s + G_j},
\]

(4)

The mathematical description of the change in the concentration of the extracted component in the suspension can be presented in the form of the following differential equation:

\[
\frac{da_j}{d\tau} = \frac{1}{\tau_{ave}} \left[ a_j^{in} - a_j^{out} \right],
\]

(5)

After transformation, taking into account (4), we have:

\[
G_j^{out} = G_j^{in} + \left[ 1 - a_j^{in} \right] \cdot G_s,
\]

(6)

\[
V_s \cdot \rho_s \frac{da_j}{d\tau} = G_s \cdot a_j - \left[ G_j^{in} \left( 1 - a_j^{in} \right) \cdot G_s \right] \cdot a_j \cdot a_j^{out},
\]

(7)

where \( a_j^{in}, a_j^{out} \) - respectively, the concentration of the extracted component in the suspension at the inlet and outlet. The mathematical description reflecting the rate of change in concentration in the liquid phase can be represented as:

\[
V_s \cdot \rho_s \frac{da_j}{d\tau} = G_j^{in} \cdot a_j^{in} + G_j^{e}a_j^{e} - G_j^{out} \cdot a_j^{out},
\]

(8)

where \( G_j^{e}, a_j^{e} \) - the amount and concentration of the extract in the solid phase.

After transformation taking into account (6) and expression
we have the following equation

\[ V_s \cdot \rho_s \frac{d a_s}{d \tau} = \left[ G_j = \frac{1}{(1 - a_s^m a_s^m)} \cdot G_s a_s^k \right] \cdot \left[ G_j^m + (1 - a_s^m) G_s \right], \]

when compiling a mathematical model of the extraction process of coniferous plants, the influence of temperature among. The change in the amount of heat in the liquid phase is described by the differential equation:

\[ \frac{d Q_j}{d \tau} = q_s + q_j^{in} - q_j^{out}, \]

where \( q_s \) - heat inflow with a suspension, \( q_j^{in} \)-heat inflow with a liquid phase, \( q_j^{out} \)-heat carried away by the liquid phase.

The amount of heat is determined from the expression:

\[ q_s = G_s \cdot C_s \cdot t_s \]

where \( G_s \) -specific heat capacity of the suspension, \( t_s \)-temperature of the suspension. The heat inflow with the liquid phase is equal to:

\[ q_j^{in} = G_j^{in} \cdot C_j^{in} \cdot t_j^{in}, \]

where \( G_j^{in} \)-specific heat of the liquid phase at the inlet, \( t_j^{in} \) is the temperature of the liquid phase at the inlet.

Heat carried away by the liquid phase

\[ q_j^{out} = G_j^{out} \cdot C_j^{out} \cdot t_j^{out}, \]

Taking into account (6), equation (14) has the form:

\[ q_j^{out} = \left[ G_j^{in} + (1 - a_s^m) G_s \right] C_j^{out} \cdot t_j^{out}, \]

where \( C_j^{out} \) - specific heat of the liquid phase at the outlet of the apparatus, \( t_j^{out} \) is the temperature of the liquid phase at the outlet of the apparatus.

Taking into account (12), (13), (15), equation (11) has the form:

\[ \frac{V_j \rho_j}{G_j \cdot C_j} \frac{d t_j}{d \tau} = G_s C_s t_s + G_j^{in} C_j^{in} t_j^{in} - \left[ G_j^{in} + (1 - a_s^m) G_s \right] C_j^{out} \cdot t_j^{out}, \]

Mathematical description of the change in the concentration of the extracted component in the solid phase. The change in the concentration of the extracted component in a solid particle depending on the radius (size) of the particle arriving for processing is described based on Fick's second law:

\[ \frac{\partial a_s}{\partial \tau} = D_\alpha \frac{\partial^2 a_s}{\partial r^2}, \]

where \( D_\alpha \) - internal diffusion coefficient of the extractable component.

It is known from the results of studies by the authors of [5,6] that the internal diffusion coefficient is an order of magnitude lower than the molecular diffusion coefficient of the extracted component in the solvent. The relationship between these coefficients has the form (17):

\[ D_\alpha = \alpha \cdot D, \]

where \( \alpha \)-coefficient taking into account the degree of destruction of the walls of the fiber, \( D \)-coefficient of molecular diffusion of the extractable component in alcohol.

The value of the diffusion coefficient of the extracted component was determined by the method described in [7,8]. Differential equation (17) describes the change in the concentration of the extracted component in any section of the processed needles particles, taking into account the hydrodynamic...
situation and the physical properties of the solvent (alcohol) being extracted. The equilibrium concentration of the extracted component in the solid particle of the needles is determined under the condition that the volume of the extracted substance occupied in the pores is filled with the extract \[9-11\]. The concentration of the extracted component in the solid phase is determined by the formula:

\[
a_k = \frac{m_k}{m_k + m_s},
\]

(19)

where \(m_k\) - the mass of the extracted substance in the solid phase, \(m_s\) is the mass of the solid particle of the needles.

The amount of the extracted substance that has passed from the solid to the liquid phase can be described by the expression:

\[
m_k = m_{ek} \cdot m_{ek},
\]

or \(m_k = V_k \cdot \rho_{ek} \cdot a_{ek}
\]

(20)

(21)

where \(a_{ek}\) - extract concentration, \(V_k\) - volume of the extracted component, \(\rho_{eq}\) is the density of the extract.

The volume of a component in the solid phase is determined by the difference between the volume of solid particles (needles) and the residual amount of solid particles of needles (after extraction):

\[
V_k = V_s \cdot V_s',
\]

(22)

In conifers germinating in the territory of Central Asia, the proportion of dissolving components is within 28-30\%. The difference according to equation (22) can be expressed as follows:

\[
V_s - V_s' = \frac{\rho_s - \rho_s'}{\rho_s} \cdot \rho_{ek} \cdot a_{ek},
\]

(23)

where \(\rho_s\) - density of a solid particle, \(\rho_s'\) is the density of a solid particle after removing the dissolving component.

Given the expression:

\[
1 = \frac{1 - a_{ek}}{\rho_{dis}} + \frac{a_{ek}}{\rho_k},
\]

(24)

where \(\rho_k\) - the density of the recovered substance.

Thus, the change in the concentration of the extractable component in the solid phase is a function of the concentration of the extractable component in the liquid phase

\[
a_k^* = f(a_{ek}),
\]

(25)

To describe the hydrodynamic structure of flows in a hydrocyclone operating in a discrete countercurrent mode, we will use the ideal displacement model. Then the change in the amount of the liquid phase at the outlet from the apparatus can be described by the differential equation in the form

\[
\frac{d_j^{\text{out}}}{d\tau} = \frac{1}{\tau_{\text{ave}}} \left[ K G_{\text{ave}}^{\text{in}} - G_j^{\text{out}} \right],
\]

(26)

where \(\tau_{\text{ave}}\) - average residence time of particles in a hydrocyclone, \(K\) is the hydrocyclone separation factor, \(G_{\text{ave}}^{\text{in}}\) - the cumulative amount of slurry and solvent at the inlet to the hydrocyclone, \(G_j^{\text{out}}\) - the amount of the liquid phase at the outlet of the hydrocyclone.

The average residence time of the material in the hydrocyclone is determined from the expression:

\[
\tau_{\text{ave}} = \frac{V_s \rho_s}{G_s},
\]

(27)

The change in the amount of thick suspension at the outlet of the hydrocyclone is described in a similar way:
\[
\frac{da_j}{d\tau} = \frac{1}{\tau_{ave}} \left[(1 - K)G_S^{in} - G_S^{out}\right],
\]

Mathematical description reflecting the change in the concentration of the extracted extract in the liquid phase:

\[
\frac{da_j}{d\tau} = \frac{1}{\tau_{ave}} \left[a_{ek}^{in} - a_{ek}^{out}\right],
\]

where \(a_{ek}^{in}, a_{ek}^{out}\) - according to the concentration of the extract in the liquid phase at the inlet and outlet of the hydrocyclone.

After transformation, the following mathematical model of the extraction process can be obtained:

\[
\begin{align*}
G_k &= G_s^{in} \cdot a_s^{in} \\
G_p &= G_s^{in} \cdot GM \\
m_k &= \frac{\rho_s - 0.7\rho_p}{\rho_s \rho_p} \frac{1}{\rho_{dis} \rho_k} \frac{a_{ek}}{a_{ek}^{out}} \\
G_k &= G_t^{in} \cdot a_t^{in} \cdot G_{t}^{out} \cdot a_{t}^{out} \\
a_{ek}^{in} &= \frac{G_{t}^{in} a_{t}^{in} + G_{ek}^{out} a_{ek}^{out}}{G_{t}^{in} a_{t}^{in} + G_{ek}^{out}}
\end{align*}
\]

The developed mathematical model serves to optimize the extraction process and design a rational device.

3. Research results

The main effect in multistage discrete countercurrent extraction is achieved by improving the structure of the streams of interacting phases by organizing the process in a discrete countercurrent mode, processing a finely dispersed product and separating a suspension between stages.

The used extraction unit allows processing of finely dispersed needles with the lowest energy costs. To build a computer model, the algorithmic blocks were aggregated. The computer model of the extraction process in the working chamber of the installation consists of a block for calculating the process at the particle level, a block for calculating the process in the liquid phase.

On the basis of the studies carried out, an extraction unit was proposed using a finely dispersed phase of the material. Figure 1.2. shows a computer simulation of the extraction process in a discrete countercurrent installation.

Figure 1. Computer simulation of the extraction process in a discrete countercurrent installation.
When extracting fine particles of needles in the field of centrifugal forces, the extraction rate increases sharply. This is explained by the following: in our example, the product is initially subjected to pre-treatment, this in turn allows the open cell pores, as a result of which the diffusion path is shortened. As a result, the internal diffusion coefficient increases by one or two orders of magnitude, this is confirmed by the results of experimental studies.

The search for an optimal extraction system is considered on the example of choosing optimal solutions for finely dispersed systems. The results of computer simulation and calculation of the extraction process for finely dispersed materials are shown in figure 3. Where the dynamics of the start-up of installations is shown, which characterizes the change in the concentration of finely dispersed material in the apparatus of a multistage discrete-countercurrent installation. The curves from top to bottom show that during the extraction of needles particles after the first, second, third discrete countercurrent installation, the concentration of solid particles gradually decreases. And for a given residual concentration of the material, the optimal number of devices is selected. The carried out theoretical studies show that the discrete countercurrent installation is optimal for the efficient implementation of the process of extraction of conifers according to hydromodules (GM). Hydromodule is the ratio of the "solid-liquid" system. Research confirms that the hydronic module has a significant effect on the change in the concentration of the solid and liquid phases. For example, with a hydromodule GM = 1: 3, within 3 hours after stage I of the installation, the concentration of solid particles decreases by 22%, after stage II to 15%, after stage III of 12%, and after stage IY of the installation, the concentration of the final product is 0.5%.

**Figure 3.** Varying the concentration of conifers over time on I, II, III, IY stages of installation.
Research shows that an increase in the diffusion coefficient $D = 2.78 \cdot 10^{-7} \frac{m^2}{c}$ has a positive effect on the rate of extraction [9-10]. The process of reaching an equilibrium state takes about 4 hours. This allows us to neglect the rate of mass transfer in its particles when modeling the process in this particular case.

4. Conclusions
In existing continuous apparatuses, heat and mass transfer processes during the counter movement of interacting flows are organized mainly in the field of gravitational forces. When extracting finely dispersed systems in a gravity field, significant difficulties arise associated with the impossibility of organizing a countercurrent flow of finely dispersed systems due to the entrainment of small particles by the counterflow, and when the particle size increases, the rate of diffusion processes decreases.

When the extraction process is carried out in the field of gravity, due to the inhomogeneity of the particle size distribution of the product, particles with different sizes have different speeds of movement along the internal space of the apparatus. Large particles move faster due to gravity and can quickly slip through the treatment zone without reaching the desired degree of condition, while small particles are slower, remaining inside the apparatus for a long time, despite the relative rapidity of the mass transfer process in such particles. The duration of the processing of solids imposes restrictions on the duration of the process as a whole.

Thus, the above contradictions significantly limit the possibility of carrying out the extraction process in the field of gravity.

Based on the factors identified in the simulation of the extraction process, an optimal device was developed. The study of multistage discrete-countercurrent installations with a discrete-countercurrent structure of interacting phases when organizing the extraction process makes it possible to eliminate the disadvantages of existing extraction installations. At each separate stage of these installations, direct flow of interacting streams is realized; in general, throughout the installation, the extraction process is carried out in a countercurrent mode. Multi-stage extraction allows you to bring the residual concentration of needles particles to the required standard level.

The implementation of the process in the proposed installation allows you to increase convective mass transfer by increasing the degree of flow turbulization. Thus, the extraction and the extraction time is shortened.

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