Modeling the polymer product maceration

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Abstract. The article contains a view of mass transmission simulation procedure conformably to control of manufacturing method's automation, and also is shown a simulator of polymer product maceration process, and results of developed for this simulator realization program system

1. Introduction
Modern technologies for polymeric products producing and processing include heat mass exchange procedures. [1,2]. Due to the complexity of modeling and analysis of such procedures using the mathematical model approach is necessary. Taking into account technological challenges, a new generation of computer technology and computer technology, polymers producing processes mathematical characterizations allow you to simulate in full. The process of modernization and improvement of production management polymeric products associated with the necessity of introducing an integrated automation.

2. The polymer product maceration
One of the principal features of the polymer production technology is the plasticizer’s application in the stages of preparation and formation of semi-finished items. Plasticizers provide the required plasticity and during subsequent process step are removed. The necessity to remove them from the composition of the polymer affects the entire manufacturing process of polymers in general [3], since the realization implies a complex set of successive heat mass exchange procedures involving, in particular, the removal of the ether, alcohol ousting with water and at list removing water or other types of drying [4].

The removing process of the solvent from the polymer product is responsible and prolonged [3]. In phase of dry- curing ester is removed which makes slowing the evaporation of the alcohol by water vapor saturation of the air approximately up to humidity of 70-85%. At the stage of maceration the group alcohol is removed. The maceration is based on mutual diffusion of water and alcohol [5]. The time of dry- curing and maceration is 36-40 hours.

The article considers the second phase of solvent removal process from the cylindrical shaped polymers. When the polymers maceration water is used for solvent extraction - alcohol and partly ether. At the process of polymers' maceration the water is used to remove solvent - alcohol and partly ether. Water is a medium for dissolving the polymer extracted from the element alcohol. Extraction is possible only in the case when the extractable substance's volume fraction in the dissolution medium is lower than the volume fraction of it in substance from which it is extracted. [6].
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While the process of running these simulations were considered the following characteristics of the process: increasing the volume fraction of water in the alcohol helps to remove the ether in the process of maceration, however, an excessive increase in the volume fraction of the alcohol extraction is a reason other substances and disturbance of the polymeric structure.

Kinetically extraction obeys the laws mass exchange, convection and molecular diffusion and the laws of transfer extractable substances from the solid phase into the liquid phase [8; 9; 10]. Driving force of transferring the target component is the difference in chemical potentials of its phases.

At simulation following assumptions were made: the convective transfer is disparagingly small; polymeric elements' shrinkage is ignored, because the extracted alcohol is substituted with water (main shrinkage of polymers occurs in the phase of dry-curing).

Constructed simulator consist of nonlinear differential equation in partial differential coefficient second-order in cylindrical coordinates, the first of which describes the process of transferring alcohol and the second transfer process water inside the polymeric element:

\[
\frac{\partial U_c(r,z,\tau)}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r} \left( r a_{mc} \frac{\partial U_c}{\partial r} \right) + \frac{\partial}{\partial z} \left( a_{mc} \frac{\partial U_c}{\partial z} \right) \tag{1}
\]

\[
\frac{\partial U_v(r,z,\tau)}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r} \left( r a_{mv} \frac{\partial U_v}{\partial r} \right) + \frac{\partial}{\partial z} \left( a_{mv} \frac{\partial U_v}{\partial z} \right), \tag{2}
\]

de \(r, z\) – spatial coordinates of the selected cylindrical coordinate system;

\(U_c(r,z), (U_v(r,z))\) – alcohol (water) concentration in the polymeric products;

\(a_{mc}, a_{mv}\) - the diffusion coefficient of the alcohol (water).

The diffusion coefficients depend on the temperature and mass content of the current value:

\[
a_{mc} = a_{m_c0} U^{n_1} T^{m_1}; \quad a_{mv} = a_{m_v0} U^{n_2} T^{m_2}, \quad \tag{3}
\]

Where \(T\) – temperature; \(a_{m_c0}, a_{m_v0}\) - the self-diffusion coefficients of water and alcohol;

\(n_1, n_2, m_1, m_2\) - some constants, which are calculated experimentally.

Differential equations with partial derivatives are generally countless solutions, therefore the formulation of a diffusion model of a porous material extraction grain polymer will be terminated if, in addition to the diffusion equation (1) and (2) will be [11] the condition of uniqueness - the initial and boundary conditions.

At the initial time \(\tau = 0\) the concentration distribution of alcohol and water in the polymer have some specified value (final conditions of dry-curing):

\[
U_c(r,z,0) = const = Q_c; \quad U_v(r,z,0) = const = Y_v. \tag{4}
\]

For the description of maceration the most used are boundary conditions of the first kind.

On the external boundary the conditions must be fulfilled:

\[
U_c(R,z,\tau) = U_c(R_k,z,\tau) = c(\tau) ; U_v(r,\frac{L}{2},\tau) = c(\tau) ; \quad \frac{\partial U_c}{\partial z}
|_{z=0} = 0; \quad \frac{\partial U_v}{\partial z}
|_{z=0} = 0. \tag{5}
\]

\[
U_v(R,z,\tau) = U_v(R_k,z,\tau) = 1 - c(\tau) ; U_v(r,\frac{L}{2},\tau) = 1 - c(\tau). \quad \frac{\partial U_v}{\partial z}
|_{z=0} = 0. \tag{5}
\]

\[
U_c(R,z,\tau) = U_c(R_k,z,\tau) = c(\tau) ; U_v(r,\frac{L}{2},\tau) = c(\tau) ; \quad \frac{\partial U_v}{\partial z}
|_{z=0} = 0; \quad \frac{\partial U_v}{\partial z}
|_{z=0} = 0. \tag{5}
\]
The boundary conditions (5) show the border has an alcohol solution in water with a concentration \(c(\tau)\), but the concentration of water in the solution is \(1 - c(\tau)\).

\[c(\tau) = \frac{(Q_1 - \overline{U})m_nN_n}{m_v + (Q_1 - \overline{U})m_nN_n(1 - \frac{p_v}{p_c})},\]  

(6)

where \(m_n\) - mass of the polymer, kg; \(m_v\) - mass of water, kg; \(\overline{U}\) - average integral concentration of alcohol; \(N_n\) - number of polymer cylinders in the pool; \(p_v\) - water density; \(p_c\) - alcohol density.

Alcohol mass in the pool, as well as \(\Delta m_{\text{воды}}\) - water mass, diffused into the polymer product, we find, on the basis of knowing the solution of the mikrokinetik problem - the change of alcohol and water average integral concentration.

\[\overline{U}(\tau) = \frac{1}{V} \iiint_V r \cdot \overline{U}(r,z,\tau) \, dr \, dz.\]  

(7)

Based on the model was developed numerical method of calculation [8; 11], and implemented a program complex calculation of the kinetics of the process of soaking. The resulting model of the dynamic properties adequate object. The simulation results show the effect on the number of fills, the processing time and the duration of the process from its initial temperature and solvent content. The bath module affects marginally.

[13].

The construction of mathematical models is an effective tool to study process. Simulation is also necessary to optimize processes and to create automated process control systems.

3. References

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