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MATHEMATICAL MODELLING OF CRYSTALLIZATION OF POLYMER SOLUTIONS

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Abstract. The processes of homogenization and crystallization of polymer solutions in cylindrical pipes are considered, which are described by the convective-diffusion equation with respect to the solution temperature and kinetic equations with respect to homogenization and crystallization of the polymer known as the thermokinetic nonlinear boundary value problem. A numerical-analytical iterative method for solving this problem is proposed, which consists of stepwise obtaining solutions of kinetic equations with respect to homogenization and crystallization of polymer solutions depending on the solution temperature and obtaining a solution of the convective-diffusion problem with respect to melt temperature. The accuracy of the obtained solution is determined by the norm of the difference between two adjacent iterations. The value of the crystallization coefficient, which is close to unity, determines the length of the dosing zone and the transition to the next zone – the flow of homogenized polymer into the distribution head of the extruder. The results of mathematical modelling are given.

Keywords: homogenization, integral transformations, iterative method, crystallization, mathematical model, nonlinear boundary value problem.

INTRODUCTION

The solution of the problem of polymer crystallization can be carried out on the basis of a mathematical model that describes the heat transfer processes of polymer melts and the cooling agent.

The main difference between the crystallization of polymers and the crystalliza\-tion of other types of materials (eg, metals) is that the crystallization of polymer melts is carried out in the space-time domain. With regard to the crystallization of polymer solutions in extrusion devices, the situation is complicated by the movement not only of the crystallization front, but also by the motion of the solid mixture heated to the melting temperature under the rotational motion of the screw worm. The crystallization process is phase, accompanied by the release of heat and leads to stresses. Determining the values of the coordinate $z = L$, in which the degree of crystallization becomes close to unity, determines the length of the dosing zone of the polymer, after which the polymer enters the extruder head. This factor plays a crucial role in ensuring the formation of a quality source product (for example, the quality of the insulating coating of the cable or the quality of the polyethylene film) at the outlet of the extruder.

PROBLEM STATEMENT

The goal of solving the problem of crystallization of polymer solutions is to develop an optimal strategy for cooling polymer solutions in order to reduce processing time and limit the use of excessively low cooling temperatures.

Overview of approaches to building models

A significant number of scientific and applied works [1, 6–8,10–15] are devoted to the construction of mathematical models of crystallization for various purposes.

Mathematical models of polymer crystallization in the form of a thin disk (one-dimensional model) are considered in [1, 12, 13]. The model consists of two nonlinear differential equations for the degree of crystallinity $y(r,t)$, defined as the average volume fraction of the space occupied by crystals, and the temperature field $T(r,t)$, combined using the norm of the nucleation and growth function $b_N(T)$ and $b_G(T)$, the nucleation initiation function and the aggregation $k(y)=1-y^2$ and saturation function of nuclei $\beta(y)=y(1-y)$:

$$\frac{\partial y}{\partial t}=\beta(y(r,t))b_G(T(r,t))+v_0 k(y(r,t))b_N(T(r,t));$$

$$\frac{\partial T}{\partial t}=\sigma\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}\right)+a_G\beta(y(r,t))b_G(T(r,t)).$$

In the given mathematical model of crystallization of the polymer solution, there are no connections of the determining components b_G, b_N from the temperature of the solution.

In [4], a mathematical model is considered, in which the dependence of the crystallization coefficient on the temperature of the polymer melt is specified explicitly.

In [8], the mathematical model takes into account the clear dependence of not only the crystallization coefficient, but also the polymerization coefficient, since these characteristics are interconnected.

Two macrokinetic parameters α and β, which determine the specific contribution of the polymer and crystalline phases, respectively, are introduced. The degree of polymerization $\alpha(t)$ determines the degree of completion of the polymerization process and can take values from 0 (the polymer content is 0) to 1 (all the monomer has turned into a polymer). The degree of crystallization $\beta(t)$ determines the degree of completion of the crystallization process and can take values from 0 (the content of the crystalline phase is 0) to 1 (the entire amorphous phase of the polymer has turned into a crystalline one). To quantitatively characterize the degree of completion of the phase transformation $\beta\in[0,1]$, a parameter called the relative degree of crystallinity is used.

Determination of temperature fields $T(r,z)$ and the degree of crystallinity $\beta(r,z)$ in insulation consists in the joint solution of the heat conduction equation and the kinetic equation:

$$V\frac{\partial T}{\partial z}=\frac{1}{c\rho}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\lambda\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)\right]+Q_v,\ r\in(R_g,R_{iz}),\ z\in(0,L); \quad (1)$$

$$\frac{\partial\beta}{\partial z}=\frac{1}{V}\left[K_0\exp\left(-\frac{U}{RT}-\frac{\psi T_{iz}}{T(T_{iz}-T)}\right)\right](1+C_0\beta)[\beta_p(T)-\beta]; \quad (2)$$

$$r \in (R_g, R_{iz}),\ z \in (0, L),\quad Q_v = \frac{VQ_m}{c}\frac{\partial\beta}{\partial z}.$$

The problem is solved under appropriate boundary and initial conditions. Note that the equations (1), (2) are written relative to the processes in the insulation, and the boundary conditions contain the conditions for the current-conducting core. In addition, the equation for the degree of crystallization is written relative to the variable , that is, a stationary problem is considered.

The presented mathematical model of polymer crystallization refers, according to the authors, to the processes of applying polymer insulation to a conductive core. However, the process of crystallization of the polymer solution is carried out even before the insulation is applied to the core, that is, in the dosing zone of the extruder. Therefore, such an approach to the study of the crystallization process of polymer solutions cannot be considered to correspond to the essence of the matter. For this reason, the mathematical model does not take into account the convective transfer of the polymer melt during the cooling process in the dosing zone.

Formulation of the problem

Assuming that technological stresses do not affect the temperature and flow of the crystallization process, it is necessary to solve the problem of determining the temperature fields and the degree of homogenization and crystallization, or the thermokinetic problem.

The problem of determining temperature fields and the degree of polymerization and crystallization is described by the following boundary value problem:

$$c(T)\rho(T)\left[\frac{\partial T(x,t)}{\partial t} + v_r\frac{\partial T}{\partial r} + v_z\frac{\partial T}{\partial z}\right];$$

$$= \operatorname{div}(\lambda(T)\operatorname{grad}T(x,t)) + \left(Q_\alpha\frac{d\alpha}{dt} + Q_\beta\frac{d\beta}{dt}\right);\quad x \in V;$$

kinetic equation of polymerization

$$\frac{d\alpha(t)}{dt} = K_\alpha(1-\alpha)(c_0+\alpha); \tag{3}$$

kinetic equation of crystallization

$$\frac{d\beta(t)}{dt} = K_\beta(T)(A_0+\beta)(\alpha\beta_p(T)-\beta); \tag{4}$$

$$K_\alpha = k_\alpha\exp\left(-\frac{U}{RT}\right);\ K_\beta = k_\beta\exp\left(-\frac{E}{RT} - \frac{\Psi T_p}{T_p - T}\right); \tag{5}$$

$$b_0 = E/R,\ b_1 = \Psi - b_0.$$

Initial and boundary conditions:

$$\alpha(x,0) = 0;\ \beta(x,0) = 0,\ T(x,0) = T_0; \tag{6}$$

$$\lambda(T)n\cdot\operatorname{grad}T(x,t) = h(T(x,t) - T_{av});\ n\cdot\operatorname{grad}T(x,t) = 0,\ x \in S_2; \tag{7}$$

$$T(x,t)=T^{*}(x,t);\;\; x\in S_1, \tag{8}$$

where c is the specific heat capacity; ρ — density; λ — thermal conductivity coefficient; Q_α, Q_β — intensities of heat sources due to polymerization and crystallization, respectively; R — universal gas table; $U, E, k_\alpha, k_\beta, c_0, c_1$ — kinetic steels determined experimentally from calorimetric measurements; melting point; β_p — equilibrium degree of crystallization;

$$\beta_b = 0{,}52\sqrt{1-(T/T_p)^4} \approx \frac{0{,}26}{T_p^2}(T_p^4 - T^4) = E_1(T_p^4 - T^4).$$

Thermophysical properties of low density polymer (PENG):

$$c = 2{,}4\ \cdot kJ/(kg^\circ\mathrm{C}));\ \lambda = 0{,}182\ \ W/(m^\circ\mathrm{C});$$

$$T_p = 170^\circ\mathrm{C};\ \rho = 1080\ \mathrm{kg/m}^3;\ T_c = 60^\circ\mathrm{C}.$$

Taking into account the fact that at the melting temperature of the polymer, the thermophysical coefficients can be considered constant, the differential equations describing the processes of heat release in the dosing zone, taking into account the smallness of the gradients relative to the axial component of the speed of movement of the polymer solution, take the form:

$$\frac{\partial v_z}{\partial t} + v_r\frac{\partial v_z}{\partial r} + v_z\frac{\partial v_z}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \mu_e \Delta v_z + g_z; \tag{9}$$

$$c\rho\left[\frac{\partial T}{\partial t} + v_r\frac{\partial T}{\partial r} + v_z\frac{\partial T}{\partial z}\right] = \lambda\Delta T + Q_\alpha\frac{d\alpha}{dt} + Q_\beta\frac{d\beta(t)}{dt}. \tag{10}$$

Initial and boundary conditions:

$$\alpha(r,z,t)\,|_{t=0} = 1,\ \ \beta(r,z,t)\,|_{t=0} = 0;\ \ T(r,z,t)\,|_{t=0} = T_p;$$

$$\left[\frac{\partial T}{\partial r} - h_0(T-T_0)\right]|_{R_1} = 0;\ \left[\frac{\partial T}{\partial r} + h_1(T-T_0)\right]|_{R_2} = 0.$$

Cooling channel:

$$v_z\,|_{z=0} = f_2(r);\ \ \frac{\partial v_r}{\partial r}|_{r=0} = 0,\ \ \frac{\partial v_z}{\partial z}|_{r=0} = 0.$$

On hard surfaces for the components of the agent that cools, meet the conditions of adhesion and impenetrability.

In the equations, the following are indicated: λ — thermal conductivity coefficient; Q_α — thermal effect of polymerization; Q_β — the thermal effect of crystallization (the rate of specific heat release during PENG crystallization); k_α, k_β — polymerization and crystallization rate constants; U — activation energy of the polymerization process; Ψ — characteristic temperature of the polymer; R — universal gas table; h_0, h_1 — coefficients of heat exchange with the environment; $T_p = 415$ K is the equilibrium melting temperature.

PROBLEM SOLVING

So, we have a system of differential equations (9), (10), (3), (4) with respect to the temperature of the polymer melt and the degree of homogenization α and crystallization β with the corresponding initial and boundary conditions (6)–(8).

This system of equations is nonlinear, its solution will be sought by an iterative scheme by analogy with the previous sections.

Let's consider the equations regarding the degree of polymerization and the degree of crystallization β. At the same time, at the first stage, we consider, $K_\alpha \sim k_\alpha$, $K_\beta \sim k_\beta$.

Since these equations contain a nonlinear component relative to $T(r,z,t)$, the exponent must be approximated, for example, by a fractional-rational expression [16]. Let's denote $e_0 = U/R$. Then we will have

$$K_\alpha(T) \approx k_\alpha\left(1-\frac{e_0T}{e_1+e_2T+e_3T^2}\right) = k_\alpha\frac{e_1-e_2T+e_3T^2}{e_1+e_2T+e_3T^2};$$

$$e_1 = e_0^2/12, \quad e_2 = e_0/2, \quad e_3 = 1.$$

By analogy, we approximate K_β in (6) $b_0 = E/R$, $b_1 = \Psi - b_0$).

$$K_\beta = k_\beta \exp\left[-\frac{b_0+b_1T}{T(T_p-T)}\right] \approx k_\beta\frac{d_0+d_1T+d_2T^2+d_3T^3+d_4T^4}{c_0+c_1T+c_2T^2+c_3T^3+c_4T^4}. \tag{11}$$

Consider the equation (3) and denote

$$N_\alpha = -\frac{1}{e_1}T\left[(e_2+T)\frac{d\alpha}{dt}-(e_2-T)k_\alpha(1-\alpha)(c_0+\alpha)\right].$$

Then we will have

$$\frac{d\alpha}{dt} = k_\alpha(1-\alpha)(c_0+\alpha)+N_\alpha(\alpha,T). \tag{12}$$

We get the solution of the equation (12) without taking into account $N_\alpha(\alpha,T)$:

$$\frac{d\alpha^{(1)}}{dt}+k\alpha = k-k_\alpha\alpha^2, \quad k = k_\alpha c_0; \quad \alpha(0)=0.$$

The solution of this equation in the first approximation:

$$\alpha^{(1)}(t) = \frac{1}{c_0}[(2kt+1)e^{-kt}-e^{-2kt}-1].$$

Further iterations in determining the expressions for the solutions in this form leads to a significant increase in the exponential terms in the solution, which actually makes it impossible to use the iterative procedure.

Therefore, it is worth now to apply the simplification algorithm and obtain the following solution of the equation (12):

$$\alpha^{(1)}(t) \approx A_2 + e^{-\gamma_\alpha t}[\bar{a}_0 f_1(\omega_\alpha t)+\bar{a}_1 f_2(\omega_\alpha t)]. \tag{13}$$

Now further iterations to determine the expression for the polymerization coefficient can be implemented according to the standard algorithmic procedure [16].

Let's go back to the expression (12). It contains an expression for the melting temperature of the polymer:

$$v_r(r,z,t)=\sum_{n=1}^{M}R_n(r)\sum_{k=1}^{N}Z_k(z)vr_{n,k}(t);\;\; v_z(r,z,t)=\sum_{n=1}^{M}R_n(r)\sum_{k=1}^{N}Z_k(z)vz_{n,k}(t)\,;$$

$$T(r,z,t)=\sum_{m=1}^{M}\sum_{k=1}^{N}R_m(r)Z_k(z)tt_{n,k}(t)\,;$$

$$tt_{n,k}(t)=t1_{n,k}^{0}-e^{-t1_{n,k}^{4}t}(t1_{n,k}^{1}f_1(t1_{n,k}^{5}t)+t1_{n,k}^{2}f_2(t1_{n,k}^{5}t)). \tag{14}$$

This expression is obtained in [17]. Application of integral transformations by spatial variables gives:

$$\overline{\overline{N_\alpha^{(1)}}}(t)=\int_{r_2}^{r_2+\alpha}R_n(\beta r)R_{n_1}(\beta r)\int_{z_0}^{L}Z_k(\delta_k z)Z_{k_1}(\delta_{k_1}z)N_\alpha(r,z,t)drdz.$$

Substituting the expression for the melt temperature in the image space by the spatial variables in gives:

$$\overline{\overline{N_\alpha^{(1)}}}(t)=\sum_{n_1,k_1}\overline{\overline{tt}}_{n_1,k_1}(t)\left[\left(\overline{\overline{tt}}_{n_1,k_1}(t)-e_2\right)\alpha^{(1)}-\left(\overline{\overline{tt}}_{n_1,k_1}(t)+e_2\right)\frac{d\alpha^{(1)}}{dt}\right].$$

Substituting (13) and (14) into this expression, performing the corresponding transformations gives

$$\overline{\overline{N_\alpha^{(1)}}}(p)\approx\frac{N_2}{p}+\frac{N_0+N_1p}{N_3+N_4p+p^2}\to\overline{\overline{N}}_\alpha^{(1)}(t)=$$

$$=na_0+e^{-na_4t}(na_1f_1(na_5t)+na_2f_2(na_5t).$$

Taking into account (13)

$$\alpha^{(2)}(t)=\alpha^{(1)}(t)+\overline{\overline{N}}_\alpha^{(1)}(t)=A_0^{(2)}+e^{-A_4^{(2)}t}(A_1^{(2)}f_1(A_5^{(2)}t)+A_2^{(2)}f_2(A_5^{(2)}t)).$$

In Fig. 1, 2 graphs of the distribution of the proportion of melt homogenization at fixed time values are given. It can be seen that the distribution of the homogenization (and crystallization) process is evened out due to the decrease in the temperature of the polymer melt.

In the space of originals by spatial variables:

$$\alpha(r,z,t)\approx\sum_{n,k}R_n(\beta_n r)Z_k(\delta_k z)\times$$

$$\times\left[A_{n,k}^{0}+e^{-(x\gamma_\alpha)_{n,k}t}(A_{n,k}^{1}f_1((\omega_\alpha)_{n,k}t)+A_{n,k}^{2}f_2((\omega_\alpha)_{n,k}t))\right]. \tag{15}$$

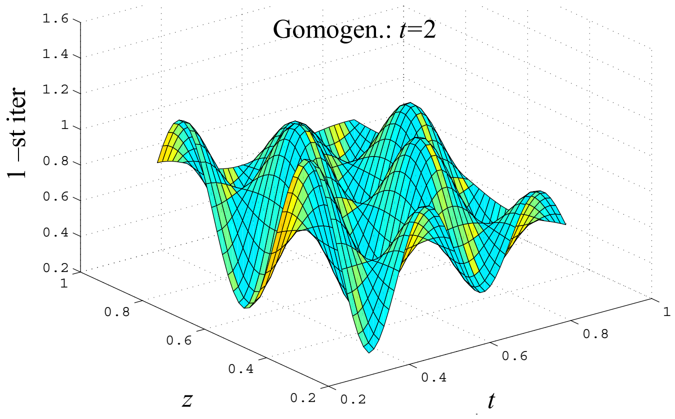

Fig. 1. Graph of distribution of polymer melt homogenization at the 1st iteration

Taking (11) into account, the equation (4) for determining the degree of crystallization takes the form

$$(c_0 + c_1T + c_2T^2 + c_3T^3 + c_4T^4)\frac{d\beta(t)}{dt} =$$

$$= (d_0 + d_1T + d_2T^2 + d_3T^3 + d_4T^4)(E_0 + \beta))[\alpha(t)E_1(T_p^4 - T^4) - \beta];$$

$$E_1 = 0{,}26/T_p^2.$$

$$c_0\frac{d\beta(t)}{dt} = d_0(e_0 + e_1\beta + e_2(\beta)^2) + N_\beta(T,\beta); \qquad (16)$$

$$N_\beta(T,\beta) = T(d_1 + d_2T + d_3T^2 + d_4T^3)(e_0 + e_1\beta + e_2\beta^2)\,.$$

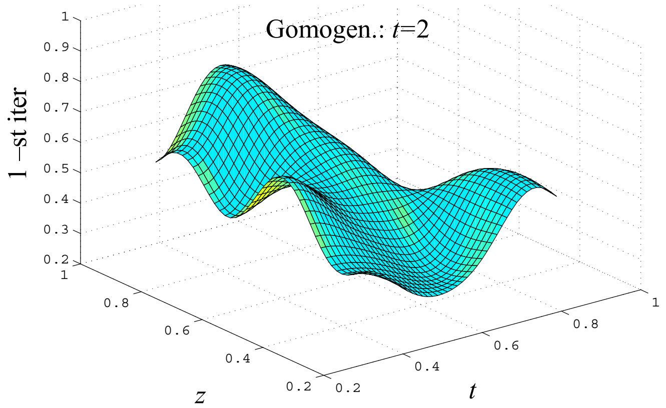

Fig. 2. Distribution graph of polymer melt homogenization at the 3rd iteration

$$-T(c_1 + c_2T + c_3T^2 + c_4T^3)\frac{d\beta(t)}{dt}. \qquad (17)$$

By analogy with (13) we obtain the solution of the equation (16)

$$\beta^{(1)}(t) \approx b_0 + e^{-\gamma_\beta t}[\bar{b}_1 f_1(\omega_\beta t) + \bar{b}_2 f_2(\omega_\beta t)].$$

In the next step, we will add to the obtained solution the dependence on the temperature of the melt $T(x,t)$, perform the transformation for $N_\beta(T,t)$ according to (17). Due to the algorithms of equivalent simplification, the solution of the equation (16) can be written in the form

$$\beta(r,z,t)=\sum_{n,k} R_n(\beta_n r)Z_k(\delta_k z)\times$$

$$\times\left[B^0_{n,k}+e^{-(\gamma_\beta)_{n,k}t}\left(B^1_{n,k}f_1((\omega_\beta)_{n,k}t)+B^2_{n,k}f_2((\omega_\beta)_{n,k}t)\right)\right].$$

Now we need to define an expression for

$$L_T=Q_p\frac{d\alpha(t)}{dt}+Q_{cr}\frac{d\beta(t)}{dt}.$$

Taking into account the obtained solutions regarding the degree of polymerization and crystallization and the calculation of the time-dependent ones, we have:

$$L_T=Q_p e^{-\gamma_\alpha t}[-(\gamma_\alpha A_0+\omega_\alpha A_1)(\omega_\alpha t)+(\omega_\alpha A_0-\gamma_\alpha A_1)(\omega_\alpha t)]+$$

$$+Q_{cr}e^{-\gamma_\beta t}[-(\gamma_\beta B_0+\omega_\beta B_1)(\omega_\beta t)]+(\omega_\beta B_0-\gamma_\beta B_1)(\omega_\beta t)].$$

We have

$$F^T_{n,k}(t)=f_0^{n,k}+e^{-\gamma_f^{n,k}t}[f_1^{n,k}(\omega_f^{n,k}t)+f_2^{n,k}(\omega_f^{n,k}t)].$$

Therefore, the temperature field of the polymer in the cooling zone is determined by the expression:

$$T(r,z,t)=T_{\text{pol}}(r,z,t)\approx\sum_{n=1}^{M}\sum_{k=1}^{M}R(\delta_n r)Z(\beta_k z)F^T_{n,k}(t).$$

The coefficients in these expressions are calculated using the appropriate C program.

Calculations were performed for the following values of the problem parameters:

$$c=57{,}3\,k\text{J/(kg}^\circ\text{C)};\ \rho=1{,}1\cdot10^3\ \text{kg/m}^3;\ \lambda_0=2{,}14848\cdot10^{-2}\,\text{kJ/(m c}^\circ\text{C)};$$

$$Q_n=4{,}297\,\text{J/(sm}^3);\ Q_{kr}=8{,}3552\,\text{J/(sm}^3);\ k_\alpha=0{,}83\,1/c;\ k_\beta=0{,}041\,1/c;$$

$$U=0{,}0443\,kJ/kg;\quad A=10^2;\ R=8{,}314;\Psi=45^\circ\text{C};\ E=0{,}034\,kJ/kg.$$

In fig. 3 shows the graph of the distribution of the fraction of crystallization for a fixed value of time.

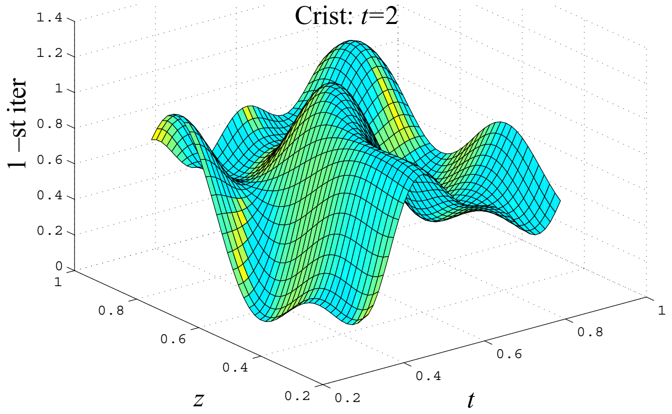

Fig. 3. Distribution graph of polymer melt crystallization on the 3rd iteration

CONCLUSIONS

1. The purpose of mathematical modeling of polymerization and crystallization processes was to determine the equilibrium state of these processes and to determine the length of the dosing zone.
2. The problem of determining the degree of polymerization and crystallization of the polymer melt in the dosing zone of the extruder is formulated in the form of a system of nonlinear differential equations with respect to the temperature of the melt (mass and heat transfer equations), taking into account the cooling boundary conditions and nonlinear kinetic equations of the degree of polymerization and crystallization of the polymer melt.
3. The solution of the system of equations of motion of the polymer melt (thermal conductivity) and kinetic equations of the degree of polymerization and crystallization is carried out by a numerical-analytical iterative method, which made it possible to obtain a solution in quadrature.
4. The distribution of the temperature of the melt crystallizing in the dosing zone, the degree of polymerization and crystallization of the polymer are obtained.
5. The proposed numerical analytical method for solving nonlinear differential equations made it possible to automate the software implementation of the iterative procedure and obtain an approximate solution for the distribution of the crystallization field of polymer solutions. Four iterations were performed to achieve a relative solution error of 5%.
6. The proposed iterative numerical analytical method proved the effectiveness of its application to a wide range of problems described by systems of nonlinear equations of the parabolic type.

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INFORMATION ON THE ARTICLE

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МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ КРИСТАЛІЗАЦІЇ РОЗЧИНІВ ПОЛІМЕРІВ

/ К.Х. Зеленський

Анотація. Розглянуто процеси гомогенізації та кристалізації розчинів полімерів у циліндричних трубах, які описуються рівнянням конвективно-дифузійної залежності від температури розчину та кінетичними рівняннями з гомогенізації та кристалізації полімера, відомими як термокінетична нелінійна крайова задача. Запропоновано числово-аналітичний ітераційний метод розв'язування цієї задачі, який полягає в поетапному отриманні розв'язків кінетичних рівнянь з гомогенізації та кристалізації розчинів полімерів залежно від температури розчину та отримання розв'язку конвективно-дифузійної задачі щодо температури розплаву. Точність отриманого розв'язку визначається нормою різниці двох сусідніх ітерацій. Значення коефіцієнта кристалізації, близьке до одиниці, визначає довжину зони дозування і перехід до наступної зони – потоку гомогенізованого полімера в розподільну головку екструдера. Наведено результати математичного моделювання.

Ключові слова: усереднення, інтегральні перетворення, ітераційний метод, кристалізація, математична модель, нелінійна крайова задача.