Mathematical Modeling of Polymer Loading Process in Extruders

K. Zelensky, Ev. Nastenko, V. Bolhovitin, O. Pavlov

Abstract: Based on the state of the problem related to high-quality and reliable insulation coating of high-voltage cables, the problems of mathematical modeling of pre-cesses in the loading zone and the delay of the polymer mixture in a single-screw extruder are formulated, which is crucial in terms of providing a high-quality insulation coating. An iterative numerical-analytical method for solving the corresponding nonlinear boundary value problems is proposed, based on the use of finite integral transformations in the spatial and temporal domains and their implementation.

Keywords: Bessel functions, extruder, integral transformations, mathematical model, numerical-analytical method, Navier-Stokes equation, polymer, screw.

I. INTRODUCTION

Due to the high productivity of the extruders, their substantial value, and the high cost of polymeric materials, experimental studies on equipment upgrades and technological regimes lead to costly materials and time costs. This leads to the development of theoretical foundations of the processes under study. One of the main tools that helps to get the results you need and allows you to minimize expensive field tests is mathematical modeling. Although the vast majority of theoretical work on the description of processes of heat transfer is based on the classical Navier - Stokes equations [1,2,3], at the same time, existing approaches to the modification of the processes of flow, heat exchange and phase transformation of polymers in channels of extrusion equipment [4] do not provide a qualitative and quantitative analysis of the processes, since the vast majority of them are formulated either in one-dimensional formulation [5-11] or formulated in three-dimensional formulation, but the corresponding boundary-value problems are not given or solved communications link to know “ standard ” packages numerical solution, which by their nature are not designed to solve nonlinear models. In addition, in our view, when setting these problems, the boundary conditions inherent in such a complex physical phenomenon are incorrectly formulated [4]. In addition, a number of problems have not been solved in the theory of plastic extrusion. As a rule, the rheological states of the polymer mixtures are not taken into account, the effect of the heat transfer processes in the auger on the processes of plastic extrusion are practically not considered.

II. METHODOLOGY AND MATERIALS

II.1 Object description

In Fig. 1 [5], provides a diagram of an extruder for coating plastic wires.

![Fig 1. Schematic of single screw extruder](image)

The object of this study is the loading zone and the delay zone in which the polymer mixture is heated to a temperature close to the melting point of the polymer. The main source of heating of the body of the extruder is induction heating. The density of internal heat sources is the electromagnetic energy released per unit time per unit volume. Due to the surface effect, the distribution of internal heat sources is significantly heterogeneous and depends on the electrophysical properties of the load, which change during heating. The whole process of heating is divided into intervals, in each of which the loading properties are assumed unchanged.

$$L(m) = \{0.9;1.45;2.05;2.65\}.$$

II.2 Heating the extruder housing

The distribution of the temperature field of the body $T_k$ is described by the equation of thermal conductivity, which in the cylindrical coordinate system has the form

$$\frac{\partial T_k}{\partial t} = a_k \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_k}{\partial r} \right) + \frac{\partial^2 T_k}{\partial z^2} \right),$$

where $a_k = \frac{\lambda_k}{c_k \rho_k}$ is the coefficient of thermal conductivity; $\lambda_k, c_k, \rho_k$ is the coefficient of thermal conductivity (W/ (m °C)), the specific heat and density of the body material, respectively; $g(r, z)$ is the function of the density distribution of the internal energy sources in the material, W / m $^3$. Given that the depth of penetration...
of electromagnetic energy from the inductor is small, \( \Delta \ll 1 \), we assume that it acts on the outer surface of the housing \( r = r_4 \). Then the boundary conditions for the housing:

\[
T_k \big|_{r=0} = T_{0k}; \quad \frac{\partial T_k}{\partial r} \big|_{r=r_4} = -\frac{q_k}{h_i} ;
\]

\[
\left[ \frac{\partial T_k}{\partial r} + h_i(T_k - T_{0k}) \right] \big|_{r=r_4} = g(r_4, z),
\]

\[
\left[ \frac{\partial T_k}{\partial z} - h_i T_k \right] \big|_{z=0} = T_0, \quad \left[ \frac{\partial T_k}{\partial z} + h_i T_k \right] \big|_{z=L} = 0.
\]

where \( h_i = \alpha_k \lambda_k \); \( \alpha_k \) is the heat transfer coefficient of the enclosure into the environment. For the contact surface of a steel pipe with air \( \alpha_k = 9 \text{ W/(m}^2 \cdot \text{C}) \).

Substitution \( T = T_k - T_{0k} \) reduces the problem to the equation

\[
\frac{\partial T}{\partial \tau} = \alpha_r \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right)
\]

with boundary conditions

\[
T \big|_{r=0} = 0; \quad \frac{\partial T}{\partial r} \big|_{r=r_4} = -\frac{q_k}{\lambda_k} ;
\]

\[
\left[ \frac{\partial T}{\partial r} + h_i T \right] \big|_{r=r_4} = g(r_4, z),
\]

\[
\left[ \frac{\partial T}{\partial z} - h_i T \right] \big|_{z=0} = (1-h_i) T_{0k},
\]

\[
\left[ \frac{\partial T}{\partial z} + h_i T \right] \big|_{z=L} = h_i T_{0k}.
\]

The values of thermophysical parameters for the housing (steel) at temperature \( T = 300K \) are equal to: \( \rho = 7845 \) kg/m\(^3\), \( c_p = 0.461 \) kW/(kg \cdot°C), \( \lambda = 58 \), \( \alpha = 10.5 \text{ K} \). Find the temperature field of the body of the extruder on the first section of heating (the area of polymer loading).

II.3 Simulation of Polymer Temperature Field in Loading Area

When formulating the boundary value of the process of heating the dry polyethylene mixture at the loading area, it is necessary to take into account the presence of a rotational motion of the screw at a constant speed \( V_m \) with cutting at an angle \( \varphi \). The heat transfer equation looks like:

\[
\rho_p c_p \left( V_m \frac{\partial T}{\partial \tau} + V_m \frac{\partial T}{\partial z} + \frac{\partial^3 T}{\partial z^3} \right) = \lambda_m \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right).
\]

For polyethylene, \( c_p \) is essentially dependent on the heating temperature [4]. The heat capacity coefficient is approximated by the dependence

\[
c_p = c_0 + c_1 T + c_2 T^2 \approx 2.5 - 0.024 \cdot T + 5.7 \cdot 10^{-4} \cdot T^2.
\]

At the boundary of the housing and the auger, the condition of equality of heat flows must be fulfilled

\[
\frac{\partial T}{\partial r} \big|_{r=r_3} = \frac{\partial T}{\partial r} \big|_{r=r_5}.
\]

Given (7) we have a boundary condition at \( r = r_3 \) for the screw temperature:

\[
T_k \big|_{r=r_3} = \frac{M}{M} \sum_{n=1}^{M} \sum_{k=1}^{M} \frac{1}{|R_k|} \left[ I_0(\beta_n r) - D_n J_0(\beta_n r) \right] \big|_{r=r_3}.
\]
\[
\times Z_t(\delta_z z) \frac{G_{nt}}{(\eta_{nt})} \left(1 - e^{-\eta_{nt} t} \right)
\]
\[
T_{sn} \bigg|_{z=0} = T_m^0,
\]
\[
\left[ \frac{\partial T_{sn}}{\partial z} + h_x T_{sn} \right] \bigg|_{z=l_z} = 0.
\]
The temperature field of the polymer mixture in the loading zone is described by the boundary value problem (8) - (13). Given the dependence of the coefficient of thermal capacity of the polymer on the temperature \(c_{vp}\), the thermal conductivity equation for the polymer in the loading zone can be written as:
\[
\frac{\partial T_p}{\partial t} = a_p \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_p}{\partial r} \right) + \frac{\partial^2 T_p}{\partial z^2} \right] + NT_p(r, z, t),
\]
where \(a_p = \lambda_p / (\rho c_{v0})\).
\[
NT_p(r, z, t) = \left[ c_1 T_p + c_2 T_p^2 \right] \frac{\partial T_p}{\partial t},
\]
where \(c_1 = -c_{n1}/c_{v0} \), \(c_2 = -c_{n2}/c_{v0} \).
Since the equation (1) is nonlinear, we will look for an iteration scheme. Solution of the linear part of the equation
\[
\frac{\partial T_p^{(0)}}{\partial t} = a_{00} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_p^{(0)}}{\partial r} \right) + \frac{\partial^2 T_p^{(0)}}{\partial z^2} \right],
\]
The difference is the condition at the boundary \(r = r_3\), which gives the expression for the temperature field at that boundary (11). When applying integral transforms for spatial variables to a boundary-value problem (14) - (16), we take into account (11) the following condition:
\[
\overline{T}^n(r_3, \gamma_k, t) = \sum_{n=1}^{M} \left[ I_0(\beta_n r_3) - D_n(\beta_n r_3) J_0(\beta_n r_3) \right]
\]
\[
\times \left[ \sum_{n_1=1}^{M} \sum_{k_1=1}^{N} \sum_{k=1}^{M} UG_{n_1, k_1, k} \left(1 - e^{-\eta_{nt} t} \right) \right]
\]
Using this expression as a boundary condition for solving the problem of heat transfer (14), (12), (13) and (17) results in operations with \(M \times N \times N\) components of appearance
\[
UG_{n_1, k_1, k} \left(1 - e^{-\eta_{nt} t} \right),
\]
making it virtually impossible to use them again. So let's simplify this expression.
\[
\overline{T}^n(r_3, \gamma_k, t) = \sum_{n_1=1}^{M} \sum_{k_1=1}^{M} \sum_{k=1}^{N} UG_{n_1, k_1, k} \left(1 - e^{-\eta_{nt} t} \right)
\]
\[
= \sum_{n=1}^{N} \sum_{k=1}^{M} \left[ g r_{n,k}^n \right] \left(1 - e^{-\eta_{nt} t} \right) + e^{-\eta_{nt} t} \left[ g r_{n,k}^n \sin(\omega_{nt} t) + g r_{n,k}^n \cos(\omega_{nt} t) \right].
\]
The algorithm behind this simplification is outlined in the section. The error that naturally arises from such simplification is offset by an iterative process when solving a nonlinear problem. Write the heat transfer equation in the screw (the temperature field of the polymer mixture) after applying the transformations on the spatial variables \(z, r\):
\[
\overline{T}_{0,n,k}(t) + \eta_{nt} T_{n,k}(t) = g z_{n,k} + G r_{n,k}(t).
\]
We will have \(t\) in image space
\[
\overline{T}_{0,n,k}(p) = \frac{1}{p + \eta_{nt} \eta_{nk}} \left[ g z_{n,k} \right]
\]
\[
\left( g r_{0,n,k} \omega - g r_{n,k} \omega + g r_{n,k} (p + \alpha_{nt}^k) \right)
\]
\[
= \frac{g z_{n,k}}{p} + \frac{t_0 n,k + t_0 k}{\eta_{nk} \eta_{nk} + t_0 n,k + t_0 n,k + p^2 s z_{n,k}}
\]
In the space of originals we have
\[
T^{(0)}(r, z, t) = \sum_{n=1}^{N} \sum_{k=1}^{M} R_{n,k}(r) Z_k(z) T^0(t).
\]
\[
T^0(t) = g z_{1,n,k} + e^{-\alpha_{nt} t} \left[ t_0 n,k \sin(\omega_{nt} t) + t_1 n,k \cos(\omega_{nt} t) \right]
\]
This expression takes into account approximate equality
\[
1 \frac{t_0 n,k + t_0 n,k}{p + \eta_{nk} \eta_{nk} + t_0 n,k + t_0 n,k + p^2}
\]
\[
= e^{-\alpha_{nt} t} \left[ t_0 n,k \sin(\omega_{nt} t) + t_1 n,k \cos(\omega_{nt} t) \right]
\]
After obtaining the solution of the equation in the form (21), taking into account (22), we will look for the solution of the equation (14) according to the iterative scheme. Recall that
\[
N T^{(1)}(r, z, t) = \left[ c_1 T_p + c_2 (TT^{(1)})_p \right] \frac{\partial T_p}{\partial t},
\]
The general scheme for solving the nonlinear equation is written in the form
\[
T^{(m)}_{p}(r, z, t) = T^{(0)}(r, z, t) + N T^{(m-1)}_{p}(r, z, t), m = 1, 2, \ldots \)
We replace the expression (20) with (15).
\[
T^{(0)}_{p} \frac{\partial T^{(0)}_{p}}{\partial t} = \sum_{n=1}^{M} \sum_{k=1}^{M} \sum_{k_1=1}^{N} R_{n_1} \left( \beta_{n_1}^k r \right) Z_{k_1} (\delta_{p})_{k_1} t
\]
\[
= \sum_{n=1}^{M} \sum_{k=1}^{M} R_{n} \left( \beta_{n}^k r \right) Z_{k} (\delta_{p})_{k} t
\]
\[
M \sum_{n=1}^{M} \sum_{k=1}^{M} \sum_{n_1=1}^{N} UG_{n_1, k_1, k} \left(1 - e^{-\eta_{nt} t} \right)
\]
\[
= \sum_{n=1}^{M} \sum_{k=1}^{M} \left( g r_{n,k}^n \sin(\omega_{nt} t) + g r_{n,k}^n \cos(\omega_{nt} t) \right).
\]
Mathematical Modeling of Polymer Loading Process in Extruders

\[
T^{(1)}_{nk}(p) = T^{(0)}_{nk}(p) + \frac{1}{p} \left[ d_1 \left( \frac{1}{p + s^3} - \frac{1}{p + s^2} \right) + d_2 \left( \frac{1}{p + s^3} + \frac{1}{p + s^5} \right) \right]
\]

(20)

The expression in square brackets \((20)\) omits (for clarity) the sums of the indices \(n_1, n_2, n_3\) and \(k_1, k_2, k_3\). For one "point", the inverse Laplace transform to \((20)\) gives the expression:

\[
T^{(1)}_{nk}(t) = T^{(0)}_{nk}(t) + \sum_{i=1}^{5} E_i e^{-\eta_t t} + \sum_{i=1}^{5} E_i e^{-\lambda_i t},
\]

(21)

Summation by the indices of the right-hand side of the equation \((31)\) will result in such an expression with respect to the operator \(p\), which makes it impossible for its practical implementation by means of computer engineering. For the solution in the second approximation we have to substitute in \((29)\) which will result in the production of expression expressions \((31)\), etc., that is, the increase of constituents relative to elementary chains in geometric progression.

This leads to the development of algorithms that prevent this growth. The accumulated errors can be compensated by additional iterations in the corresponding algorithm. So, let's go back to the equation \((31)\) and consider the expression in square brackets, taking into account thsummation of the index \(k_3\)

\[
\sum_{k_2} d_{k_1} \left( \frac{1}{p + s_{k_2}} - s_{k_2} \right) \sum_{k_2} d_{k_1} \left( \frac{1}{p + s_{k_2}} + s_{k_2} \right)
\]

\[
\approx \frac{b_{k_1} + b_{k_1} p}{b_0 + b_{k_1} + b_{k_1} p^2}.
\]

In turn, the resulting expression can be approximated by the same pattern

\[
\sum_{k_1} d_{k_1} \frac{b_{k_1} + b_{k_1} p}{c_0 + c_{n_1} + c_{n_1} p^2}.
\]

Given that the eigenvalues of \(\eta^2\) increase quite rapidly with increasing \(N\) and \(M\), we can restrict ourselves to \(N = M = 4\). An algorithm for such simplified fractional expressions is given in the section that results in:

\[
D_{nk}^{(0)}(p) = \sum_{nk} d_{nk}^{(0)} + d_4^{(0)} \frac{p}{z}.
\]

This expression corresponds to the original (in the space of integral transformations by spatial variables)

\[
D_{nk}^{(0)}(t) = \sum_{nk} e^{-\eta t} (e_{nk} f_1 \omega_{nk} t + e_{nk} f_2 \omega_{nk} t).
\]

Then the solution in the first approximation will take the form

\[
T^{(1)}(r, z, t) = \sum_{nk} R(\delta, r) Z(\beta, z)
\]

(19)

Recall that due to the notation introduced, the coefficients \(d_{1, 2}, s_i, i = 1, 5\), depend on the eigenvalues of the spatial variables. Apply to the Laplace transform equation over time (the initial condition is zero). We have:
formulation is called enthalpy. The domain $\Omega^+(t)$ of the liquid phase, where the temperature exceeds the phase transition temperature $T^+$, is 

$$\Omega^+(t) = \{(x, y, z) | \text{in} \Omega, T(x, y, z) > T^+\}.$$  

Similarly, for the speed of free bound.


t Stefan condition (ref stef.05) x, z)) + f^-, (x, y, z) \in Q^- \}$.

Given the convective transfer in the liquid phase,

$$c^+ \rho \left( \frac{\partial T^+}{\partial t} + v \text{grad} T^+ \right) = \text{div}(k^+ \text{grad} T^+) + f^+, (x, y, z) \in Q^+.$$  

where $[\cdot]$ denotes a jump in the boundary of the $S$ phase transition.

The phase transition is accompanied by the release / absorption of a certain amount of heat. Therefore, the thermal flux at the boundary of the phase transition is discontinuous and is determined by the magnitude

$$\left[ \frac{\partial T}{\partial n} \right] = -L V_n, (x, y, z) \in S.$$  

Here $L$ is the enthalpy of the phase transition, $V_n$ the velocity of the phase transition boundary at normal.

At the boundary of the phase transition conditions of the first kind are fulfilled:

$$T(x, y, z, t) = T^+, (x, y, z) \in S(t).$$  

Conditions (37)-(39) -- Stefan conditions, and the corresponding problem for the equations (35), (36) is called the Stefan problem. From the point of view of constructing efficient algorithms, it is important that the Stefan problem admits a generalized formulation under which the conditions (37)-(39) are included in the thermal conductivity equation itself.

$$c_\rho \left( \frac{\partial T}{\partial t} + v \text{grad} T \right) = \text{div}(k \text{grad} T) + f, (x, y, z) \in Q.$$  

Near the boundary of the phase transition, we introduce a local orthogonal coordinate system $(x', y', z')$, whose metric coefficients are equal to one. In these new coordinates, the surface $\delta$ - function $\delta_\delta$ is

$$\delta_\delta = \delta(x' - x_0'),$$

where the equation $x' = x_0'$ defines the limit $S$. Similarly, for the speed of free boundary motion we have

$$V_n = dx'/dt.$$  

The Stefan condition (ref stef.05) corresponds to the fact that in the new coordinates $T = T(x', y', z', t), T(x', y', z', t) = T^*.$

$$\delta_\delta V_n = \delta(x' - x_0') \frac{dx'}{dt} = \delta(T - T^*) \frac{dT}{dt}.$$  

(30)
Substituting (ref stef.10) into (ref stef.09) gives the desired equation

\[ [\epsilon \rho + L \delta(T - T^*)] \left( \frac{\partial T}{\partial t} + v \nabla T \right) = \text{div}(k \nabla T) + q_v. \]

Considering the phase transition heat is equivalent to setting the effective heat capacity:

\[ c_{ef} = c + \frac{1}{\rho} L \delta(T - T^*). \]

\[ \rho c_{ef} \left( \frac{\partial T}{\partial t} + v \nabla T \right) = \text{div}(k \nabla T) + q_v, \]  \[ (32) \]

The iterative procedure for solving the given system of equations is as follows.

1. First, we obtain the solution of the linearized equation corresponding to

\[ \rho \left( \frac{\partial v^{(0)}}{\partial t} + \mu \frac{\partial^2 v^{(0)}}{\partial z^2} \right). \]

2. The solution obtained for the velocity \( v^{(0)}(z,t) \) to solve the equation of the linear part of the equation with respect to temperature

\[ \rho c_{0v} - LT^* \left( \frac{\partial T^{(0)}}{\partial t} + v^{(0)} \nabla T^{(0)} \right) \]

3. Find the solution of the equation taking into account the dependence of the heat content coefficient on the melt temperature \( c_{0v} + L(T - T^*) \cdot T^{(1)}(z,t) \).

4. Determine the expression for pressure using

\[ p = \rho R T^{(1)}(z,t). \]

5. We obtain the solution of the equation (44) in the first approximation, that is, we solve the equation

\[ \rho \left( \frac{\partial v^{(1)}}{\partial t} + \mu \frac{\partial^2 v^{(1)}}{\partial z^2} \right) - N_v(v^{(0)}, T^{(1)}) = \text{div}(k \nabla T) + q_v. \]

6. Repeat steps 2–5 until \( | \vec{v}^{(m+1)}(z,t) - T^{(m)}(z,t) | > \Delta \) with the indexes 0 and 1 replaced by \( m \) and \( m+1 \).

### III. RESULTS AND DISCUSSION

Mathematical modeling of the processes of heating of the screw housing and the polymer mixture in the loading zone and the delay zone is performed. The solutions of the nonlinear boundary value problems of heat transfer in the loading zone and the delay are obtained, taking into account the nonlinear properties of the coefficient of heat capacity and convective transfer of speed in the delay zone. An algorithm for solving the problem of moving boundaries of the solid and liquid phases of a polymer is proposed.

### IV. CONCLUSION

The problem solved, in our opinion, is essential for solving the problem of optimal heating of the polymer mixture in terms of providing high-quality insulating coating of the cable to ultra-high voltages.

### REFERENCES


AUTHORS PROFILE


Under the guidance of C. Zelensky are defended 4 and 3 dissertations are being carried out for the degree of Candidate of Technical Sciences in the specialty “Computer Sciences”.

Evgen Nastenko, Doctor of Biological Sciences, Senior Researcher, Head of the Department of Biomedical Cybernetics, Faculty of Biomedical Engineering, National Polytechnic University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”. Member of the Specialized Scientific Council 14.01.04 - Cardiovascular Surgery of the State Institution “National M. Amosov” Institute of Cardiovascular Surgery”. Member of the Specialized Scientific Council 03.00.20 - Biotechnology, Faculty of Biotechnology and Biotechnologies. Igor Sikorsky Kyiv Polytechnics Institute. Head of scientific projects: 1. Development of a robust method for automatic identification of anatomical features of the heart for cardiac analysis. Samsung Electronics Ukraine Company. Contract dated 26.06.2014.r. 2. Blood pressure assessment. Samsung Electronics Ukraine Company. Contract dated 09.10.2018. 3. “Methods and Models for the Identification of the State of Biological Objects” (2017-2022) He has 306 publications, of which 284 are scientific, 3 chapters in three monographs, 13 patents, including 156 scientific papers published in national and international peer-reviewed professional journals, 17 articles in Scopus. Under the guidance of Dr. E.A. Nastenko are defended 6 and 2 dissertations are being carried out for the degree of Candidate of Technical Sciences in the specialty "Computer Sciences".