The emergence of bifurcation phenomena during the flow of rheologically complex media in a tubular reactor

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Annotation. The mathematical model describing heat-mass transfer in the course of rheologically complex media in a tubular reactor is developed in the article. Using the example of the continuous production scheme for grade B2 polymethacrylate, solutions of the characteristic equations confirming the possibility of emergence of critical flow regimes for certain sets of control parameters were obtained.

Introduction

In 1928 Academician N.N. Semenov published a paper describing a phenomenon later called "thermal explosion in gas media". In the 30s - 40s of the XX century a great development in the study of this subject was made by such prominent scientists as: O.M. Todes, D.A. Frank-Kamenetsky and Ya.B. Zeldovich.

In 1965, Bostanjinyan S.A., Merzhanov A.G. and Khudyaev S.I. [1] equations analogous to the equations proposed by Semenov were obtained, but already for the flow of a viscous Newtonian fluid. The later investigations of the flow of viscous fluids do not give an exhaustive answer to the question of the appearance of conditions under which a progressive increase in temperature arises.

In the mathematical models available to date, the non-Newtonian properties of liquids are not taken into account and there are no methods for calculating the qualitative characteristics by means of the molecular mass distribution.

In connection with the need to solve various applied problems arising during the design and operation of thermal power plants, the task of theoretical research of heat and mass transfer processes in the laminar flow of Newtonian, decontaminating and pseudoplastic chemically reacting liquids in pipes and channels has come to the fore.

Statement of the problem

In this paper, the flow of rheologically complex media in a tubular reactor is considered. A closed mathematical model describing heat and mass transfer in the course of fluid motion inside a tubular reactor is developed, which reflects the mutual influence of hydrodynamic, heat-mass exchange, rheological and macrokinetic parameters on the polymerization process.

As a working agent (monomer) in the reactor, a polymethacrylate of grade B2 is considered, which releases heat as a result of its absolute mixing with the initiator.
In constructing the mathematical model, the following assumptions were made:
1. the flow of the laminar steady-state reaction system with the generated profile of the velocity vector at the inlet to the reactor;
2. mass forces enter the equations of motion implicitly, but through excess pressure;
3. the transfer of heat and mass along the direction of the main motion due to thermal conductivity is small in comparison with the forced transfer in the same direction;
4. the thermophysical characteristics of the system and the coefficients of mutual diffusion change insignificantly during the reaction;
5. The hydrodynamic relaxation time is much shorter than the thermal time, i.e. the profile of the velocity vector almost instantly adapts to the change in the temperature field;
6. the system under investigation does not possess elastic properties.

For the study, the system of equations of motion, energy conservation, the continuity equation and the mass transfer equations recorded for the monomer and initiator were used [2]. As a rheological model, was chosen a power-law model [4].

The system of equations under study is as follows:

\[
\rho \left( \frac{\partial V_i}{\partial t} + \frac{\partial V_j}{\partial z} \right) V_i = 2 \mu \left( \frac{\partial \mu}{\partial t} \right) + \frac{\partial P}{\partial z} + \mu \left( \frac{\partial \mu}{\partial z} \right) - 2 \mu V_i + 2 \mu \frac{\partial V_i}{\partial z} \]

\[
\rho \left( \frac{\partial V_j}{\partial t} + \frac{\partial V_j}{\partial z} \right) V_j = \frac{\partial}{\partial t} \left( \frac{\partial V_i}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\partial V_i}{\partial z} \right) + 2 \frac{\partial}{\partial z} \left( \frac{\partial V_i}{\partial z} \right) - \frac{\partial P}{\partial z} + \mu V_j + \mu \frac{\partial V_j}{\partial z} \]

\[
\frac{\partial V_i}{\partial t} + \frac{V_i}{r} + \frac{\partial V_j}{\partial z} = 0
\]

\[
V_i \frac{\partial T}{\partial t} + V_j \frac{\partial T}{\partial z} = \alpha \left( \frac{\partial^2 T}{\partial t^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) + \frac{Q_s k_m}{c_m} e^{E_R T} M^n J^n + \frac{2 \mu I_2}{\rho c_p}
\]

\[
V_i \frac{\partial M}{\partial t} + V_j \frac{\partial M}{\partial z} = D_m \left( \frac{\partial^2 M}{\partial t^2} + \frac{1}{r} \frac{\partial M}{\partial r} \right) - k_s e^{E_R T} M^n J^n
\]

\[
V_i \frac{\partial J}{\partial t} + V_j \frac{\partial J}{\partial z} = D \left( \frac{\partial^2 J}{\partial t^2} + \frac{1}{r} \frac{\partial J}{\partial r} \right) - k_J e^{E_R T} J
\]

\[
I_2 = \left( \frac{\partial V_i}{\partial t} \right)^2 + \frac{1}{2} \left( \frac{\partial V_i}{\partial z} + \frac{\partial V_j}{\partial z} \right)^2 + \left( \frac{V_i}{r} \right)^2 + \left( \frac{\partial V_j}{\partial z} \right)^2
\]
Not considering $\frac{\partial P}{\partial r}$ and taking into account $Q = \left[ \int V_r \, d\Omega = \int_0^{2\pi} \int_0^{\infty} V_r \, r \, dr \right]$, we have:

$$\frac{\partial P}{\partial z} = \frac{2\pi r}{Q} \left[ 2V_z \frac{\partial}{\partial z} \left( \mu \frac{\partial V_z}{\partial z} \right) - \mu \left[ \frac{\partial V_z}{\partial r} + \left( \frac{\partial V_z}{\partial r} \right)^2 \right] \right] dr$$

Thus, in order to study the flow of a rheologically complex liquid in a tubular reactor, taking into account the Stokes assumption, we have the following system of equations:

$$\left\{ \begin{array}{l}
\frac{2\pi r}{Q} \left[ 2V_z \frac{\partial}{\partial z} \left( \mu \frac{\partial V_z}{\partial z} \right) - \mu \left[ \frac{\partial V_z}{\partial r} + \left( \frac{\partial V_z}{\partial r} \right)^2 \right] \right] dr = \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \left[ \frac{\partial V_z}{\partial z} + \frac{\partial V_z}{\partial r} \right] \right) + 2 \frac{\partial}{\partial z} \left( \mu \frac{\partial V_z}{\partial z} \right) \\
\frac{\partial V_z}{\partial r} + \frac{V_z}{r} + \frac{\partial V_z}{\partial z} = 0 \\
V_z \frac{\partial \xi}{\partial r} + V_z \frac{\partial \xi}{\partial z} = \rho \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) + \frac{Qo k_o e^{E/RT} M^a J^a}{\rho c_p} + 2 \mu I \frac{\partial J}{\partial r} \\
V_z \frac{\partial M}{\partial r} + V_z \frac{\partial M}{\partial z} = \rho \left( \frac{\partial^2 M}{\partial r^2} + \frac{1}{r} \frac{\partial M}{\partial r} \right) - k_o e^{E/RT} M^a J^a \\
V_z \frac{\partial J}{\partial r} + V_z \frac{\partial J}{\partial z} = \rho \left( \frac{\partial^2 J}{\partial r^2} + \frac{1}{r} \frac{\partial J}{\partial r} \right) - k_o e^{E/RT} J^a \\
I = \left[ \frac{\partial V_z}{\partial r} + \frac{1}{2} \left( \frac{\partial V_z}{\partial z} + \frac{\partial V_z}{\partial r} \right)^2 \right] + \left( \frac{V_z}{r} \right)^2 + \left( \frac{\partial V_z}{\partial z} \right)^2 
\end{array} \right.$$
and considering the power model as a rheological model:

\[ \mu = \mu_0 I_1^2 = A \cdot e^{\frac{B}{RT}} \cdot I_1^2 \]

we have:

\[
\frac{2\pi r_1^4}{Q^2} \int_0^1 \left[ 2V_r \frac{\partial}{\partial z} \left( e^{\frac{a_1}{\beta \theta}} \cdot I_1^2 \cdot \frac{\partial V_z}{\partial z} \right) - e^{\frac{a_0}{\beta \theta}} \cdot I_1^2 \cdot \left( \frac{\partial V_z}{\partial x} + \frac{(\partial V_x)}{\partial x} \right)^2 \right] dx =
\]

\[
= \frac{1}{x} \frac{\partial}{\partial x} \left( e^{\frac{a_0}{\beta \theta}} \cdot I_1^2 \cdot \left( \frac{\partial V_z}{\partial x} + \frac{(\partial V_x)}{\partial x} \right) \right) + 2 \frac{\partial}{\partial x} \left( e^{\frac{a_0}{\beta \theta}} \cdot I_1^2 \cdot \frac{\partial V_x}{\partial x} \right)
\]

\[
\frac{\partial V_z}{\partial x} + \frac{\partial V_x}{\partial z} + \frac{\partial V_y}{\partial t} = 0
\]

\[
\pi RT_0^2 \frac{V_t}{Q} e^{\frac{a_0}{\beta \theta}} \left( \frac{\partial V_z}{\partial x} + \frac{\partial V_x}{\partial z} \right) = \alpha \frac{RT_0^2}{Q} \left( \frac{\partial^2 V_z}{\partial x^2} + \frac{\partial^2 V_x}{\partial x \partial z} \right) + \frac{M^a \cdot \tilde{j} \cdot Q \cdot \frac{\partial \tilde{M}}{\partial t}}{Q \cdot \frac{\partial V_x}{\partial \tilde{x}} - \frac{\partial \tilde{M}}{\partial \tilde{x}}} - k_0 e^{\frac{a_0}{\beta \theta}} e^{\frac{a_0}{\beta \theta}} M^a j^a
\]

Analytical study of the task

We expand all the functions under investigation into Taylor series in a neighborhood of the point \((0, z_0)\) on the channel axis and taking into account that the functions \(0, M, J, V_r\) are even relative \(x\), and the function \(V_t\) is odd.

The value of the coefficients in the expansion of the function \(V_t\) is found from the continuity equation. Functions \(I_2^1 (1 = \frac{1}{k}\) for polymers) and \(e^{\frac{a_0}{\beta \theta}}\) and \(e^{\frac{a_0}{\beta \theta}}\) decompose into Taylor series, and the function \(I_1\) does not decompose into a series (its components decompose into series) [5].

Substituting the expansion functions for the investigated functions, we obtain a system of four algebraic equations (the continuity equation is not used, because with its help the coefficients of the Taylor series for the function \(V_t\) are obtained) [6].

From the consideration of the coefficients for the free term and at \((z - z_0)\), adding initial conditions for the temperature, velocity, concentration of the monomer and initiator, we obtain a system of 16 algebraic equations \((k = 3, s = 1, m = 1, n = 1)\).

If we substitute the boundary conditions of the first kind and renumber it \(\theta_0\) for \(h\), we obtain the following characteristic equation for determining the temperature of the working agent:
\[ \theta_i = h - \frac{\delta \exp\left(\frac{h}{1 + \beta h}\right)}{4} + \frac{1}{16} \left[ -\chi \exp\left(\frac{\alpha h}{(1 + \beta h)}\right) + \frac{\delta^2 \exp\left(\frac{2h}{(1 + \beta h)}\right)}{4(\beta h + 1)^2} \right] - \]
\[
- \frac{1}{36} \left[ \chi \exp\left(\frac{\alpha h}{(1 + \beta h)}\right) \left( c_0 - 1 \right) \left( 1 - \exp\left( - c_1 \right) \right) - \frac{\alpha \delta \exp\left(\frac{h}{1 + \beta h}\right)}{4(\beta h + 1)^2} \right] + \]
\[
+ \frac{3\delta^3 \exp\left(\frac{3h}{1 + \beta h}\right)}{64(1 + \beta h)^4} - \frac{\beta \delta^3 \exp\left(\frac{3h}{1 + \beta h}\right)}{16(1 + \beta h)^3} - \frac{\chi \delta \exp\left(\frac{(\alpha + 1)h}{1 + \beta h}\right)}{16(1 + \beta h)^2} \right].
\]

Fig.1. Graphical representation of the equation with respect to polymethacrylate grade B2 10%, taking into account the dissipative and chemical source of heat release under thermal boundary conditions of the first kind for a round tube \( T_0 = 413 \text{ K}, T_1 = 418 \text{ K} \).

In the case when thermal boundary conditions of the third kind are given on the boundary, then, after re-designation \( \theta_i \) for \( h \), we obtain the following characteristic equation for determining the temperature of the working agent:

\[
144 \cdot (h - \theta_i) = 4 \left[ \chi \cdot \exp\left(\frac{\alpha h}{(1 + \beta h)}\right) \left( c_0 - 1 \right) \left( 1 - \exp\left( - c_1 \right) \right) - \frac{\alpha \cdot \delta \cdot \exp\left(\frac{h}{1 + \beta h}\right)}{4(1 + \beta h)^2} \right] + \]
\[
+ \frac{3\delta^3 \exp\left(\frac{3h}{1 + \beta h}\right)}{64(1 + \beta h)^4} - \frac{\beta \delta^3 \exp\left(\frac{3h}{1 + \beta h}\right)}{16(1 + \beta h)^3} - \frac{\chi \delta \exp\left(\frac{(\alpha + 1)h}{1 + \beta h}\right)}{16(1 + \beta h)^2} \left( \frac{6}{\text{Bi}} + 1 \right)
\]
Fig. 2. Graphical representation of the equation with reference to polymetacrylate of grade B2 10%,
taking into account the dissipative and chemical source of heat release under thermal boundary
conditions of the third kind for a circular pipe. \( T_0 = 413 \text{ K}, \ T_1 = 418 \text{ K}. \)

The conducted analysis of the behavior of the lines of solutions of the characteristic equations for
polymetacrylate of grade B2 confirms the existence of critical flow regimes for certain sets of
parameters and shows the possibility of switching to the non-calculating operating modes of heat
engineering equipment.

Conclusions

1. A method for analytical investigation has been developed and a theoretical substantiation of
the possibility of the appearance of bifurcation phenomena in the flow of a nonlinear viscous fluid in
an infinite circular tube under thermal boundary conditions of the first and third kind has been developed.

2. A technique for analytical analysis of heat and mass exchange of nonlinear viscous fluids in
tubular homophase rectilinear reactors has been developed.

3. When considering the flow of polymetacrylate grade B2 in a tubular reactor, solutions of
characteristic equations were obtained, analysis of which shows the possibility of switching to non-
calculating operating modes of heat engineering equipment for certain values of control parameters.

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