Determination of the conditions of spontaneous combustion of a rheologically complex medium inside the continuous infinite cylinder in convective heat transfer case

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Abstract. We obtain the dependence of the relative temperature of a rheologically complex medium depending on the distance to the center of the cylinder. The conditions of spontaneous combustion and the stability of the solutions obtained were investigated, and the approximations of the expressions obtained were carried out. The results obtained in this work allowed us to determine the areas of occurrence of critical flow regimes inside a hollow cylinder under thermal boundary conditions of the 1st and 3rd kind.

1 Introduction

In connection with the need to solve various applied problems arising during the design and operation of heat and power plants, the problem of theoretical study of heat and mass transfer processes during the flow of chemically reacting liquids in pipes and channels has come to the fore.

The stationary heat conduction equations in a circular pipe, in channels of complex shapes under various boundary conditions were considered in [1-5]. In [6], the construction of a mathematical model of the polymerization process in a tubular reactor was analyzed in detail.

The purpose of this work is to obtain the dependence of the relative temperature on the distance to the center of the cylinder, to identify the conditions of spontaneous combustion and to determine the stability of the solutions obtained, as well as an approximation of the expressions obtained.

2 Methods

In this paper, a mathematical model of D.A. Frank-Kamenetskii is used

$$\frac{d^2\theta}{d\varepsilon^2} + \frac{1}{\varepsilon} \cdot \frac{d\theta}{d\varepsilon} = -Fk \cdot \exp[\theta]. \quad (1)$$

This equation is a stationary heat conduction [7,8] equation of an infinite cylinder with a chemical heat source, the reaction rate of which obeys the Arrhenius law, the Frank-Kamenetskii method [9] is used for approximation.

Here:

$$\varepsilon = \frac{r}{r_1};$$

$$Ar = \frac{R \cdot T_1}{E};$$

$$\theta[\varepsilon] = \frac{T[\varepsilon] - T_1}{Ar \cdot T_1};$$

$$Fk = \frac{Q_0 \cdot K_0}{\lambda \cdot Ar} \cdot \exp\left[-\frac{1}{Ar}\right] \cdot r_1^2$$

r is the distance from cylinder axis; r_1 is the outer cylinder radius; Ar is the Arrhenius number; R is the universal gas constant; T_1 is the cylinder surface temperature; E is the activation energy of a chemical reaction; Fk is the Frank-Kamenetskii criterion; $T[\varepsilon]$ is the absolute temperature; K_0 is the chemical reaction rate constant; Q_0 is the thermal effect of a chemical reaction; λ is the coefficient of thermal conductivity.

When the cylinder is filled with a condensed phase, the walls are heated [10]. If heat transfer occurs by means of convection, then according to the model of Barzykin V. V. and Merzhanov A. G. the thermal boundary conditions of the 3rd kind are [11]

$$\begin{cases} \theta[1] + \frac{\theta'_\varepsilon[1]}{Nu} = 0, \\ \theta'_\varepsilon[0] = 0, \end{cases} \quad (2)$$

where Nu is the Nusselt criterion.

All calculations are performed using the MATHEMATICA software product [12].

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3 Results

The general solution (1) has the form:

$$\theta[\varepsilon] = \ln \left[\frac{2 c_1^2 c_2 \varepsilon^{-2+c_1}}{(\varepsilon^{c_1+c_2 Fk})^2} \right]. \quad (3)$$

Analysis of the formula (3) shows that:

1. $c_1, c_2 \neq 0$.
 2. For solid cylinder:
 - 2.1. $0 \leq \varepsilon \leq 1$;
 - 2.2. $c_1 = 2$, as otherwise $\theta[0]$ is undefined;
 - 2.3. $\theta[\varepsilon]$ monotonously decreasing when $0 \leq \varepsilon \leq 1$;
- consequently,

$$\theta[\varepsilon] = \ln \left[\frac{8 c_2}{(\varepsilon^2 + c_2 Fk)^2} \right], \quad (4)$$

$$\theta_{max} = \theta[0] = \ln \left[\frac{8}{c_2 Fk^2} \right], \quad (5)$$

where c_1, c_2 are the roots of the system, obtained by substituting (3) into thermal boundary conditions.

As (4) is an even function, it satisfies the last equation from (2). After substituting (4) into the first equation of (2) and some algebraic transformation the system (2) will have the form:

$$\ln \left[\frac{8 c_2}{(1+c_2 Fk)^2} \right] - \frac{4}{Nu (1+c_2 Fk)} = 0. \quad (6)$$

It seems to be impossible to solve this equation analytically. We denote:

$$q_2[c_2] = \ln \left[\frac{8 c_2}{(1+c_2 Fk)^2} \right] - \frac{4}{Nu (1+c_2 Fk)} \quad (7)$$

Analysis of (7) showed that:

1. $c_2 > 0$;
2. $q_2[c_2]$ has a vertical asymptote when $c_2 = 0$;
3. $q_2[c_2]$ has an extremum (max);
4. c_{2max} is the root of the equation $q_2' = 0$:

$$c_{2max} = \frac{2 + \sqrt{Nu^2 + 4}}{Nu Fk}; \quad (8)$$

$$q_{2max} = \ln \left[Nu \frac{\sqrt{Nu^2 + 4} - Nu}{Fk} \right] - \frac{4}{2 + Nu + \sqrt{4 + Nu^2}}; \quad (9)$$

4. $q_2[c_2]$ monotonously increases when $0 < c_2 < c_{2max}$
5. $q_2[c_2]$ monotonously decreasing when $c_2 > c_{2max}$,
6. $q_2[c_2]$ has no roots if

$$q_{2max} < 0. \quad (10)$$

7. $q_2[c_2]$ has the unique root if (spontaneous combustion condition):

$$q_{2max} = 0. \quad (11)$$

8. $q_2[c_2]$ has two roots if

$$q_{2max} > 0. \quad (12)$$

The graphs of $q_2[c_2]$ with different Fk and constant $Nu = 3.659$ are shown in figure 1.

Fig. 1. Graphical interpretation of equation (9) for various Fk and constant $Nu = 3.659$.

The spontaneous combustion conditions can be transformed by substitution of (9) and (11) and the subsequent solution of the obtained equation

$$Fk = Fk_{cr} = \exp \left[\frac{\sqrt{Nu^2 + 4} - 2 - Nu}{Nu} \right] * Nu (\sqrt{Nu^2 + 4} - Nu). \quad (13)$$

Analysis of (13) shows that:

1. Fk_{cr} - monotonously increases;
2. Fk_{cr} - has the horizontal asymptote

$$asimptota[Fk_{cr}] = 2. \quad (14)$$

The resulting equation coincides with the condition of spontaneous ignition of an infinite cylinder under thermal boundary conditions of the first kind [9].

To simplify the calculations, we approximate (13):

1. By fractional rational function $Pade1/1$ [13];

$$\frac{Pade1}{1[Fk_{cr}]} = 2 - \frac{8}{2 Nu + 3}; \quad (15)$$

2. By fractional rational function $Pade2/2$;

$$\frac{Pade2}{2[Fk_{cr}]} = 2 - 6 \frac{2 Nu + 1}{3 Nu^2 + 6 Nu + 4}. \quad (16)$$

The graphs of (13) - (16) are shown in figure 2

Fig. 2. Graphical Interpretation of Equations (13-16).

For numerical comparison of the approximating curves, we use the absolute value of the relative error

$$\delta[Pade1/1[Fk_{cr}]] = \left| \frac{Fk_{cr} - Pade1/1[Fk_{cr}]}{Fk_{cr}} \right|, \quad (17)$$

$$\delta \left[\frac{Pade2}{2[Fk_{cr}]} \right] = \left| \frac{Fk_{cr} - Pade2/2[Fk_{cr}]}{Fk_{cr}} \right|, \quad (18)$$

$$\delta[asimptota[Fk_{cr}]] = \left| \frac{Fk_{cr} - asimptota[Fk_{cr}]}{Fk_{cr}} \right|. \quad (19)$$

The graphs of (17) - (19) are show in figure 3.

Fig. 3. Graphical Interpretation of Equations (17-19).

By substituting (13) into (8) we can calculate the unique root of (6) with respect to (13):

$$c2_{cr} = \frac{(2 + \sqrt{Nu^2 + 4})(Nu + \sqrt{Nu^2 + 4})}{4 Nu^2} \exp \left[\frac{2 + Nu - \sqrt{Nu^2 + 4}}{Nu} \right] \quad (20)$$

$c2_{cr}$ has the horizontal asymptote

$$asimptota[c2_{cr}] = \frac{1}{2}. \quad (21)$$

$asimptota[c2_{cr}]$ coincides with $c2_{cr}$ when thermal boundary conditions of the first kind are held.

With respect to (9) the inequation (10) can be transformed:

$$Fk > Fk_{cr}. \quad (22)$$

With respect to (9) the inequation (12) can be transformed:

$$Fk < Fk_{cr}. \quad (23)$$

The equation (6) cannot be solved analytically under the conditions (22) and (23). To solve it we will use:

1) the localization of the roots by the analytical method

$$q2[c2] < 0 \text{ if } \ln \left[\frac{8 c2}{(1 + c2 Fk)^2} \right] = 0, \quad (24)$$

which gives us

$$q2[c23] < 0 \quad (25a)$$

$$q2[c24] < 0, \quad (25b)$$

where

$$c23 = \frac{Fk - 4 + 2\sqrt{2}\sqrt{2 - Fk}}{Fk^2} - \text{is the smaller root of (24),}$$

$$c24 = \frac{4 - Fk + 2\sqrt{2}\sqrt{2 - Fk}}{Fk^2} - \text{is the greater root of (24).}$$

Consequently,

$$c23 < c21 < c2_{max}, \quad (26a)$$

$$c2_{max} < c22 < c24, \quad (26b)$$

where $c21$ - is the smaller root of (6), $c22$ - is the greater root of (6).

2) The refining of localized roots.

To calculate the $c21$, $c22$ with fixed Fk , Nu we can use any of numerical methods of solving the non-linear equations [13].

By substituting the roots of (6) into (4) we get the partial solutions of (1) with respect to (2).

• If (22) is valid, then (1) has no partial solutions.

When this condition is held, according to the stationary theory [9] the stationary distribution of temperature is impossible.

• If (13) is held, then (1) has the unique partial solution.

This solution is the critical one

$$\theta_{cr}[\varepsilon] = \frac{2 + Nu - \sqrt{4 + Nu^2}}{Nu} + \ln \left[\frac{2(2 + \sqrt{4 + Nu^2})(Nu + \sqrt{4 + Nu^2})}{(2 + \sqrt{4 + Nu^2} + Nu \varepsilon^2)^2} \right] \quad (27)$$

The function $\theta_{cr}[\varepsilon]$ has the asymptote

$$asimptota[\theta_{cr}] = 2 \ln \left[\frac{2}{1 + \varepsilon^2} \right]. \quad (28)$$

By substituting (27) into (5) and performing the transformations, we get:

$$\theta_{cr max} = \frac{2 + Nu - \sqrt{4 + Nu^2}}{Nu} + \ln \left[\frac{2(Nu + \sqrt{4 + Nu^2})}{2 + \sqrt{4 + Nu^2}} \right]. \quad (29)$$

The function $\theta_{cr max}$ has the horizontal asymptote

$$asimptota[\theta_{cr max}] = \ln[4] \quad (30)$$

Taking into account the cumbersomeness of (29) we will approximate it with a fractionally rational Pade function to make it simpler [14-16].

$$Pade2/2[\theta_{cr max}] = \ln[4] - \frac{18}{18 Nu^2 + 24 Nu + 41}. \quad (31)$$

The graphs of (29) - (31) are shown in figure 4.

To compare the approximating curves, we use the absolute value of the relative error:

$$\delta[asimptota[\theta_{cr max}]] = \left| \frac{\theta_{cr max} - asimptota[\theta_{cr max}]}{\theta_{cr max}} \right|, \quad (32)$$

$$\delta[\text{Pade2/2}[\theta_{cr \max}]] = \left| \frac{\theta_{cr \max} - \text{Pade2/2}[\theta_{cr \max}]}{\theta_{cr \max}} \right|. \quad (33)$$

The graphs of (32) - (33) are shown in figure 5.

Fig. 4. Graphical Interpretation of Equations (29-31).

Fig. 5. Graphical Interpretation of Equations (32-33).

If (23) is valid, then (1) has two different partial solutions.

$$\theta_1[\varepsilon] = \ln \left[\frac{8 \cdot c_{21}}{(\varepsilon^2 + c_{21} \cdot Fk)^2} \right], \quad (34a)$$

$$\theta_2[\varepsilon] = \ln \left[\frac{8 \cdot c_{22}}{(\varepsilon^2 + c_{22} \cdot Fk)^2} \right], \quad (34b)$$

consequently,

$$\theta_{1 \max} = \ln \left[\frac{8}{c_{21} \cdot Fk^2} \right], \quad (35a)$$

$$\theta_{2 \max} = \ln \left[\frac{8}{c_{22} \cdot Fk^2} \right] \quad (35b)$$

We should note that:

3.1. $\theta_1[\varepsilon] > \theta_{cr}[\varepsilon] > \theta_2[\varepsilon]$,

3.2. $\theta_1[\varepsilon_{\max}] > \theta_{cr \max} > \theta_2[\varepsilon_{\max}]$.

The graphs of (27), (35a), (35b) are shown in figure

6.

Fig. 6. Graphical Interpretation of Equations (27), (35a), (35b).

3.3 $\theta_1[\varepsilon]$ is unstable as $\theta_1[\varepsilon_{\max}]$ when $\delta=0$ has a vertical asymptote and is decreasing monotonously (see figure 7), which is physically impossible.

Fig. 7. The dependence of the relative temperature on the value of the Frank-Kamenetskii parameter.

4 Discussion

Our research shows that:

1.If $Fk < Fk_{cr}$ (1) has two partial solutions with respect to the thermal boundary conditions (2). The greater of partial solutions is unstable.

2.If $Fk = Fk_{cr}$ (1) has the unique partial solution with respect to the thermal boundary condition (2). This solution is critical.

3.If $Fk > Fk_{cr}$, then according to the stationary theory [9] the stationary distribution of temperature is impossible.

4.Depending on the required accuracy and the value of Nu , the spontaneous combustion condition can be calculated exactly, or replaced by the spontaneous combustion condition under boundary conditions of the first kind or by the approximating fractional rational Padé function.

5. $\theta_{cr \max}$ depending on the required accuracy and the value of Nu , it can be calculated exactly, either replaced by $\lg 4$ or calculated by the approximating rational fractional Padé function.

The use of the approximating fractional rational Padé function significantly reduces the amount of calculations.

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