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Influence of Boundary Conditions on the Critical Parameters of Reactive Flow Ignition in a Channel with Heat Recuperation

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Abstract. A one-dimensional problem of reacting flow thermal stability in a U-shaped channel is studied. A finite difference scheme is proposed for this problem. Borders of domain of existence of a bounded solution are estimated. Calculations are carried out for two variants of the inlet boundary condition. Relationship between critical parameter and other parameters is obtained.

Keywords: differential equation, thermal explosion, numerical solution, recuperative heat transfer.

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Thermal explosion problems are problems with critical parameters for which the solution exists only under restrictions on values of these parameter. Frank–Kamenetsky considered classical thermal explosion problems related to the stability of reacting media [1]. The thermal stability of reacting flows which is directly related to problems of chemical and energy engineering were studied [2, 3]. The influence of forced and free convection was considered [4–9]. Thermal explosion equations contain source terms responsible for heat release (often, this is an exothermic chemical reaction, Joule heat, or viscous dissipation [10–15]) and terms responsible for heat transfer (thermal conductivity, convection). As a rule, these are local relations. Non-local transport mechanisms appear, for example, in media with radiative heat transfer [16–18] or in media of complex structure [19–21]. In this work, thermal explosion equation with non-local term is studied. It naturally appears when considering recuperative heat exchange surface in a U-shaped channel. Combustion in such channels was previously considered in many works (for example, see [22–25]).

1. Thermal explosion equation for a U-shaped channel

The classical thermal explosion problem for plane symmetry with conductive heat transfer may be written as follows [1]

$$\frac{d^2\theta}{dx^2}(\xi) + Fk \exp\left[\theta(\xi)\right] = 0. \tag{1}$$

Here θ is temperature, ξ is spatial coordinate, and Fk is Frank–Kamenetsky number (critical parameter of the problem). Frank–Kamenetsky number is defined as the ratio between heat source intensity and conductive heat transfer rate: $Fk = \dfrac{E_a L^2 Q w(T_0)}{\lambda R_g T_0^2}$ (here E_a is chemical reaction activation energy, L is a reactor size, Q is a reaction heat, T_0 is ambient temperature,

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$w(T_0)$ is reaction rate at ambient conditions, λ is thermal conductivity, R_g is the universal gas constant).

Boundary conditions are as follows

$$\frac{d\theta}{d\xi}(0) = 0; \theta(1) = 0. \quad (2)$$

The critical value of Fk is about 0.88. Equation (1) does not have a solution at higher Fk because reacting medium becomes unstable reaching high-temperature conditions when equation (1) is not applicable. In the presence of convective heat transfer (for example, in the presence of reacting mixture flow in a channel), the equation can be written in the form

$$-Pe\frac{d\theta}{d\xi}(\xi) + \frac{d^2\theta}{dx^2}(\xi) + Fk\exp[\theta(\xi)] = 0. \quad (3)$$

Here Pe is the Peclet number, $Pe = \frac{c\rho uL}{\lambda}$. Here c is heat capacity, ρ is fluid density, u is mean velocity, L is a channel length. It was shown that as Pe increases the critical value of Fk also increases reaching limit $Fk_{cr} \longrightarrow Pe$ [26]. Equation (2) is correct for small heat losses. Otherwise, it should be modified as follows

$$-Pe\frac{d\theta}{d\xi}(\xi) + \frac{d^2\theta}{dx^2}(\xi) + Fk\exp[\theta(\xi)] - Bi_{env}\theta(\xi) = 0. \quad (4)$$

Here Bi is the Biot number, $Bi = \frac{\alpha L}{\lambda}$ (α is heat transfer coefficient). Generally, the Biot number depends on the Peclet number but in this paper they are considered as independent parameters. Equation (4) describes the stationary heat transfer in one-dimensional linear channel (Fig. 1a). As the numbers Pe and Bi increase the critical value of Fk also increases [27]. The non-stationary behaviour of reacting flow was considered in [28]. In the present work, the primarily interest is in ignition conditions (how Fk_{cr} depends on conditions) rather than its dynamic features.

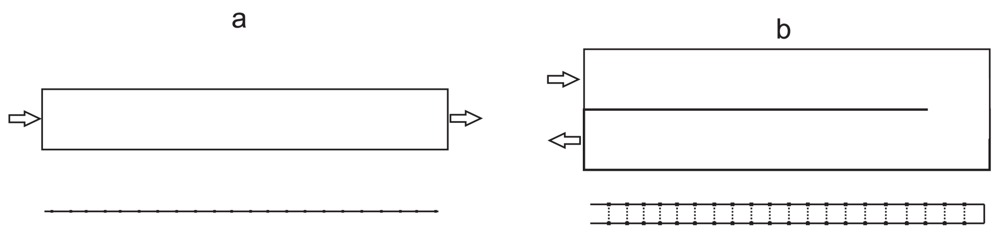

Fig. 1. Schemes of a linear channel (a) and a U-shaped channel (b). Corresponding finite difference grids are shown below plots

Let us consider a U-shaped one-dimensional channel. It is a simple model of a recuperative burner (Fig. 1b). The inner surface of such channel allows heat exchange between sections. The reaction products heat the fresh mixture which enlarges the stable combustion ranges compared with linear channels [22–25]. It is possible to represent a U-shaped channel in the form of a one-dimensional graph [29] as shown in Fig. 1b. Additional connections appear between the two halves of the channel (dashed lines). The thermal explosion equation can be written as follows

$$-Pe\frac{d\theta}{d\xi}(\xi) + \frac{d^2\theta}{dx^2}(\xi) + Fk\exp[\theta(\xi)] - Bi[\theta(\xi) - \theta(1-\xi)] = 0. \quad (5)$$

Equation (5) contains the term responsible for heat loss which is non-local, i.e., it depends on temperature at two points. With additional bending of the channel temperature dependence may become more complex.

The problem with two counterflow channels is not quite equivalent to equation (4) since equation (5) is continuous at the inflexion point while in the problem with two channels the choice of suitable boundary conditions is required [22, 23]. The critical condition for equation (5) corresponds only to the upper limit of thermal stability. Therefore it does not reflect the range of high-temperature stationary states. Our estimates have rather limited applicability. A regime map for a similar problem with two counterflow channels was presented [22, 23], where one can find several possible types of behaviour. In this paper, only the stability limit of low-temperature steady states is considered, i.e., conditions of self-ignition of reacting flow are found.
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2. Finite difference scheme

Equation (5) can be approximated with the following finite difference scheme

$$(1 + hPe)\,\theta_{i-1} - \left(2 + hPe + h^2 Bi\right)\theta_i + \theta_{i+1} + h^2 Bi\theta_{N+1-i} = -h^2 Fk \exp\left(\widetilde{\theta_i}\right). \tag{6}$$

The difference system produces system of linear equations if the right hand side is linearised or fixed. It can be solved using standard solvers.

Assuming $Bi = 0$ and expanding the exponential function in equation (5), one can obtain truncated linear differential equation that can be solved analytically to test difference scheme (6). Results of numerical solution are presented in Fig. 2. Numerical error ε is defined as the integral of absolute difference between numerical solution and exact solution, and N is a number of grid nodes. Upper graphs correspond to the equation with constant and uniform heat source:

$$-Pe\frac{d\theta}{d\xi}(\xi) + \frac{d^2\theta}{dx^2}(\xi) + Fk = 0. \tag{7}$$

Lower graphs were obtained for the linear heating source:

$$-Pe\frac{d\theta}{d\xi}(\xi) + \frac{d^2\theta}{dx^2}(\xi) + Fk\,(1+\theta) = 0. \tag{8}$$

The difference scheme is stable and approximates the original differential equation with the first order of accuracy (this is due to the convective term). Calculations show that when Peclet number is less then 100 upwind scheme does not suffer from numerical diffusion. High Peclet numbers were not considered due to requirements of laminar flow.

Stability of the difference scheme (6) is supported by fixing the right hand side (heat source). After each iteration temperature distribution is updated, and the problem is solved for updated fixed heat source. The space step $h = 0.002$ was used in the calculations. The critical value of the Fk number can be found by the bisection method as described in [30].

3. Results and discussion

It is natural to expect that when $Pe = 0$ and $Bi = 0$ the critical number Fk will be equal to 0.88. For $Bi = 0$ the relationship between Fk_{cr} and Pe was obtained in [26, 27]. Fig. 3 shows the relationship between critical value Fk and numbers Pe, Bi. As Pe increases at a constant Bi the critical value of Fk increases over almost the entire calculated region. However, in the range of Pe numbers close to 4 the relationship between Fk_{cr} and Bi changes. At lower Pe,

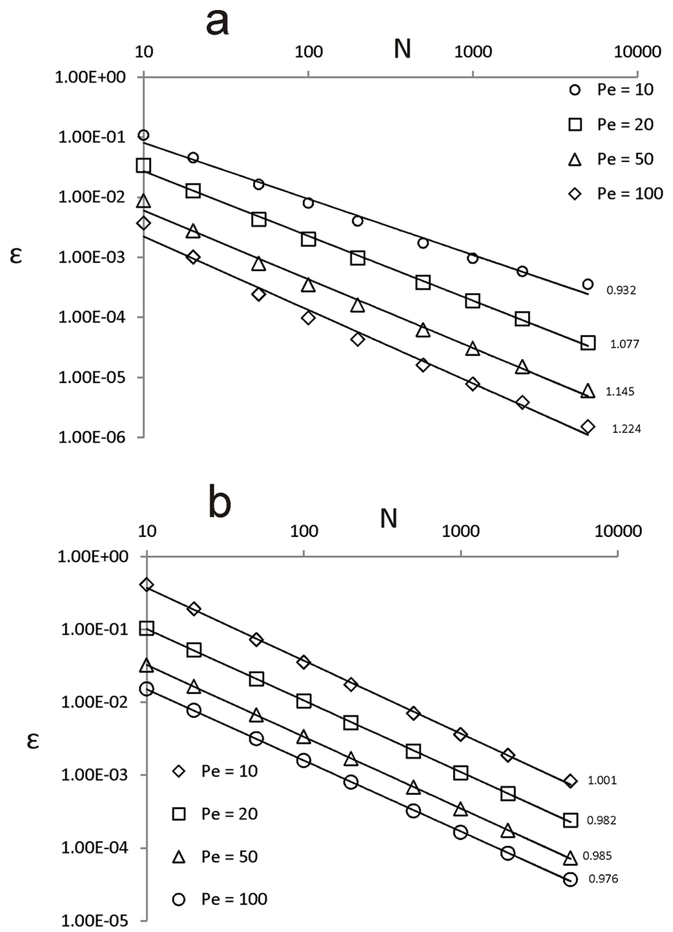

Fig. 2. Relationship between numerical error and number of grid nodes for linearised equations: (a) constant heating source; (b) linear heating source. Numbers on the right are orders of accuracy

an increase in Bi leads to an increase in Fk_{cr} and vice versa at higher Pe. It means that heat transfer intensification between the channel parts narrows the region of stable ignition for low flow rates.

Fig. 4 shows the effect of Bi in more detail. As Bi increases the values of Fk_{cr} and the maximum temperature converge to the same limit. Interestingly, for large Bi numbers the maximum temperature is reached not at the reactor outlet but in its middle, at the channel inflexion point. Fig. 5 shows the temperature profiles at the stability border. The temperature profile does not depend on Pe in the limit of large Bi. This phenomenon can be explained as follows. With high intensity of heat transfer through the inner wall of the channel the temperature distribution becomes more and more symmetrical. In this case, the critical value Fk_{cr} is equal to the critical value in the half-channel. The dimensional analysis gives the value of $0.88 \times 2^2 = 3.52$ which is close to calculated values. The maximum admissible temperature in this setting is 1.2 which is also observed from calculations.

The boundary conditions for problem (5) in form (2) are not quite correct. The inlet Dirichlet boundary condition choice leads to the situation when the main heat loss at low Pe is due to heat transfer through the inlet boundary (which corresponds to the transition region in Fig. 2). It

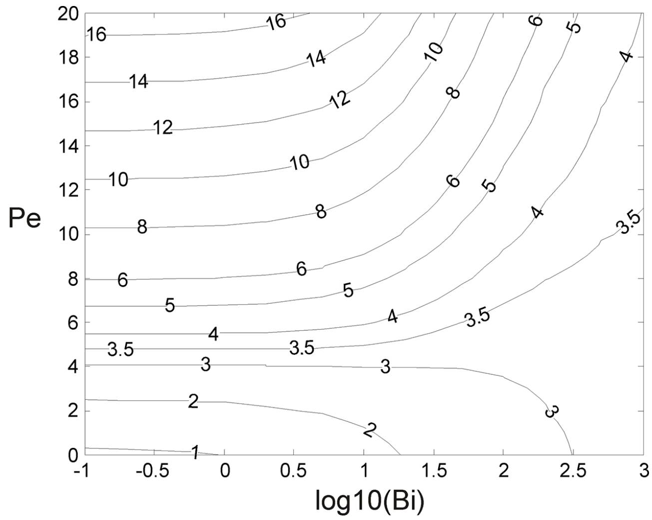

Fig. 3. Relationship between critical value of Fk (isolines) and parameters Bi, Pe under Dirichlet inlet boundary condition

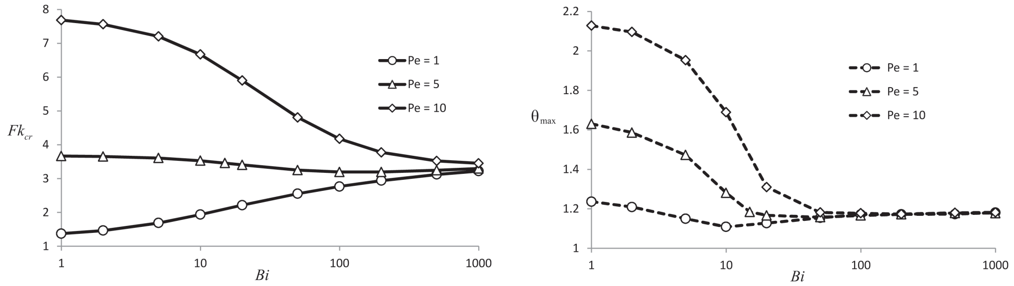

Fig. 4. Relationship between Fk_{cr}, θ_{max} and Bi under Dirichlet inlet boundary condition

means that condition (2) corresponds to the case when reactive mixture enters into the channel from a temperature-controlled reservoir. It may not quite accurately reflect the physical picture of the problem. If the reactor does not have such a control then heat flow through the left boundary may lead to a dangerous situation when preheated fresh mixture reacts before entering the channel. In this case a more reasonable choice is thermally isolated flow-permeable left boundary that is described by the Danckwerts boundary condition [31]

$$\frac{d\theta}{d\xi}(0) = -Pe\theta(0). \tag{9}$$

Fig. 6 shows the relationship between critical value Fk and Pe, Bi under boundary condition (9). This relationship is monotonic in both variables. However, for small Pe the heat loss through the inlet boundary is low so the reaction mixture ignites already at small Fk. It means that for low Pe heat recuperation occurs due to the thermal conductivity of the reaction mixture itself. In this case, the temperature near the inlet becomes close to critical. This may cause a flashback of the flame into the reservoir. Another reason for the low Fk_{cr} values is the neglect of heat losses through the outer channel walls.

Fig. 7 shows temperature profiles at the thermal stability border. As in the previous case, profiles tend to have a symmetric parabolic shape in the large Bi limit but the number Pe

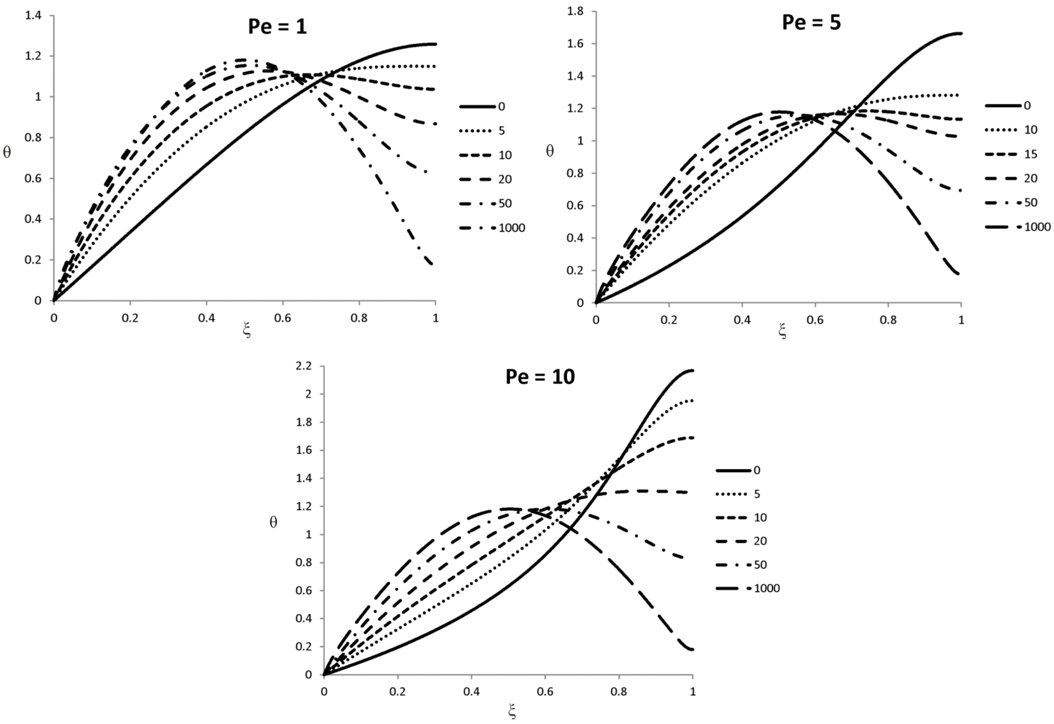

Fig. 5. Temperature profiles in U-shaped channel under Dirichlet inlet boundary condition

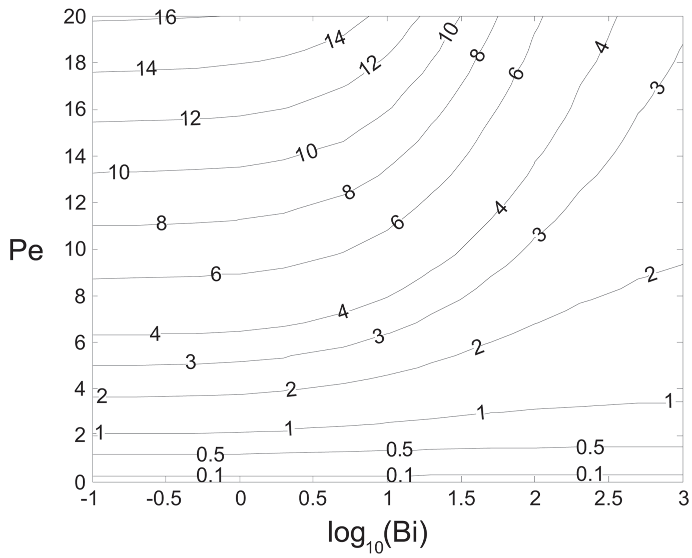

Fig. 6. Relationship between critical value of Fk (isolines) and parameters Bi, Pe under Danckwerts inlet boundary condition

included in the boundary condition determines the reaction mixture temperature at the inlet. As Pe increases the difference between solutions corresponding to boundary conditions (2) and (9) decreases. In general, as Bi increases the critical number Fk decreases (Fig. 8), i.e., the ignition region is expanding. Heat recuperation makes it possible to achieve the ignition of mixtures with a lower calorific value (although the notable effect requires heat transfer intensification by orders of magnitude).

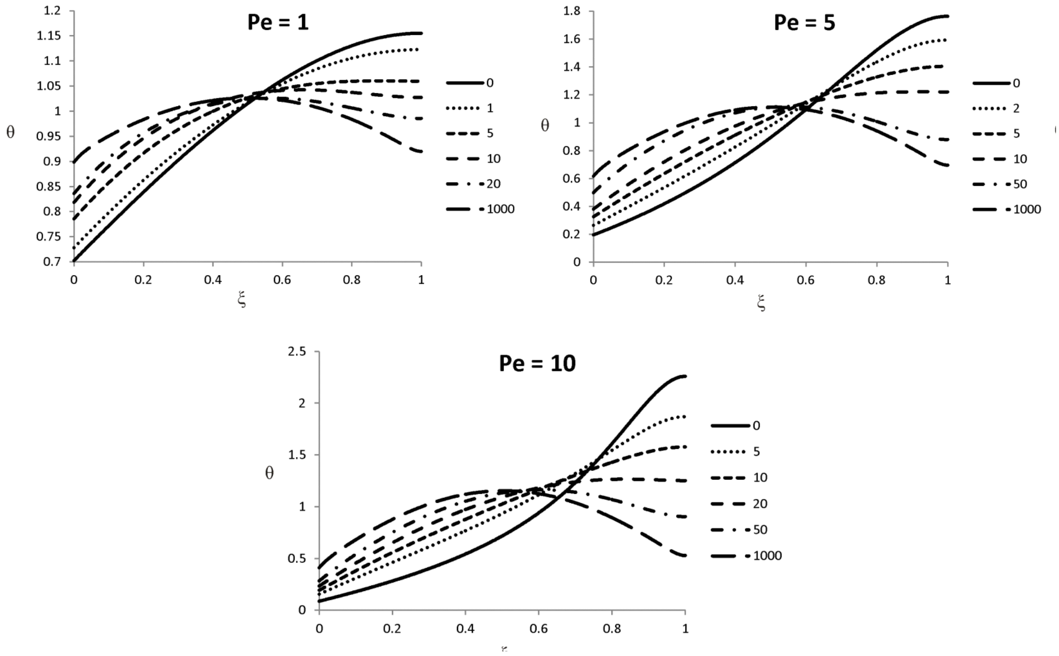

Fig. 7. Temperature profiles in U-shaped channel under Danckwerts inlet boundary condition

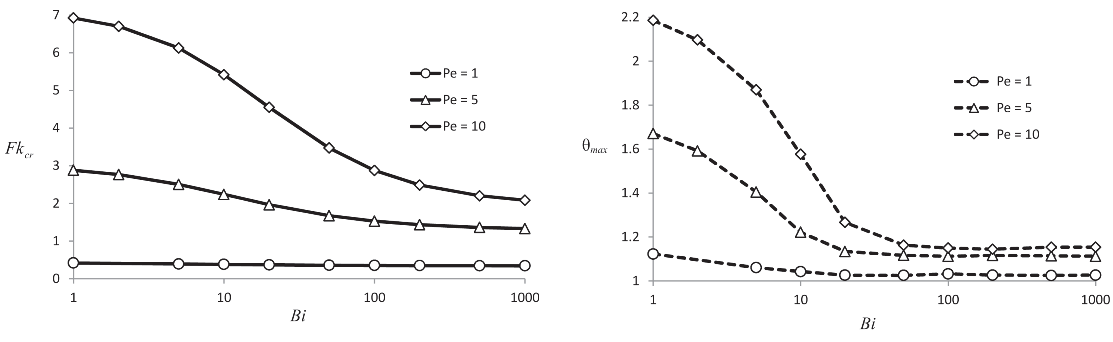

Fig. 8. Relationship between Fk_{cr}, θ_{max} and Bi under Danckwerts inlet boundary condition

It should be noted once again that applicability of the results is limited by the self-ignition phenomenon. Free variation of parameters Pe and Bi is also an approximation. In the general case, the number Bi is found from the solution of the conjugate heat transfer problem [32]. In addition, the thermophysical properties of the reacting mixture are assumed to be constant while in practice this is not the case. For example, during the combustion of gases the density is very sensitive to temperature. Since velocity is determined from the continuity equation then the velocity depends on the chemical reaction rate (such relationship may be one of the reasons for fluctuations in the combustion front). Finally, the model does not take into account the heat losses of the outer channel walls. Their presence will significantly change the regime map.

Conclusion

In this work, the behaviour of the temperature distribution in a channel with a counterflow heat transfer is numerically studied which makes it possible to recuperate the heat released during an exothermic reaction. The relationship between critical parameter Fk and the flow rate (Pe) and the heat transfer coefficient (Bi) is calculated. It is shown that when the Dirichlet inlet boundary condition is used non-physical solutions appear. This corresponds to conductive heat loss through the boundary. These solutions vanish when the Danckwerts boundary condition is used. The obtained results can be useful to study the limits of self-ignition in reactors with heat recuperation.

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Влияние граничных условий на критические параметры зажигания в реагирующем потоке в канале с рекуперацией теплоты

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Аннотация. Исследована одномерная задача тепловой устойчивости реагирующего потока в U-образном канале. Для этого предложена разностная схема решения нелокального уравнения конвективного теплопереноса. Оценены границы области существования ограниченного решения. Проведены расчеты для двух вариантов входного граничного условия. Получены зависимости значения критического параметра от расхода и интенсивности теплоотдачи.

Ключевые слова: дифференциальные уравнения, тепловой взрыв, численное решение, рекуперативный теплообмен.