Numerical modeling of 1D heterogeneous combustion in porous media under free convection taking into account dependence of permeability on porosity

N A Lutsenko

1 Institute of Automation and Control Processes FEB RAS, Vladivostok, 690041, Russia
2 Far Eastern Federal University, Vladivostok, 690950, Russia
E-mail: NickL@inbox.ru

Abstract. Using numerical experiment the one-dimensional unsteady process of heterogeneous combustion in porous object under free convection is considered when the dependence of permeability on porosity is taken into account. The combustion is due to exothermic reaction between the fuel in the solid porous medium and oxidizer contained in the gas flowing through the porous object. In the present work the process is considered under natural convection, i.e. when the flow rate and velocity of the gas at the inlet to the porous objects are unknown, but the gas pressure at object boundaries is known. The influence of changing of permeability due to the changing of porosity on the solution is investigated using original numerical method, which is based on a combination of explicit and implicit finite-difference schemes. It was shown that taking into account the dependence of permeability on porosity, which is described by some known equations, can significantly change the solution in one-dimensional case. The changing of permeability due to the changing of porosity leads to the speed increasing of both cocurrent and the countercurrent combustion waves, and to the temperature increasing in the combustion zone of countercurrent combustion wave.

1. Introduction

Heterogeneous combustion in porous media is quite common in nature. From the point of view of mechanics the porous media include peat, coal dumps, landfills, debris of destroyed buildings and so on. Heterogeneous combustion of porous objects may appear as a result of natural and man-made disasters: explosions at atomic and industrial facilities, destruction of buildings involving fires, underground explosions, peat fires, spontaneous self-ignition of solid waste dumps (landfills) and so on. In such porous objects the filtration combustion takes place under natural convection. In this case the flow rate of gas passing through the porous object is unknown and the flow rate of oxidant, which enters into the reaction zone in porous object, regulates itself. One type of heterogeneous combustion in porous media is smoldering as heterogeneous chemical reactions take place during smoldering.

There are a lot of publications devoted to both the solid porous media combustion and the gas combustion in filtration mode; general concepts and basic theory of filtration combustion were presented in the review paper [1]. Analytical investigations of counter-flow combustion of solid porous medium under free convection, when the gas and the combustion wave in porous object move in opposite directions, were carried out in [2]. The co-flow combustion of solid porous
medium under free convection, when the gas moves in the same direction as the combustion wave, was investigated analytically in [3]. In [4] the ability of energy to be concentrated in front of a co-flow filtration combustion wave in a porous solid was analyzed. In [5] it was shown that reduction of the permeability in the combustion products can lead to hydrodynamic instability of combustion wave. In [6] a one-dimensional transient model of smoldering was presented and solved numerically. A novel computational model of smoldering combustion capable of predicting both the countercurrent and the cocurrent wave propagation was developed in [7]. A generalized pyrolysis model, Gpyro, for simulating the gasification of a variety of combustible solids encountered in fires was presented in [8]. In [9], [10] Gpyro was expanded to two-dimensional case. In [11] the one-dimensional unsteady process of heterogeneous combustion in porous object under free convection in the gravity field was investigated numerically using proposed mathematical model and an original numerical method. Two regimes of combustion wave propagation have been revealed – wave movement up the object (cocurrent burning) and down the object (countercurrent burning) – which differ significantly from each other by the degree of burnout of solid combustible material, the temperature in the combustion zone and the speed of combustion wave propagation. The details of the original numerical method were described in [12]. In [13] the effects of gravity field and pressure difference at the boundaries of the porous object on the appearance of stable heterogeneous combustion waves in object under free convection were investigated numerically.

This work is devoted to the numerical investigations of one-dimensional unsteady processes of heterogeneous combustion in porous object under free convection in the gravity field when the dependence of permeability on porosity is taken into account. The proposed mathematical model is briefly described, the model is similar to the one used in [11]–[13] and allows us to describe the processes both under free convection and forced filtration. The influence of the permeability changing due to the changing of porosity on the solution is investigated using numerical experiment.

2. Mathematical model and numerical method
Consider a homogeneous motionless porous object with a height $H$, which is bounded of impermeable non-heat-conducting side walls and opened on two opposite sides (at the top and at the bottom). In the porous medium the heterogeneous reactions take place that leads to the heat release. The cold gas can flow into the open walls of the porous object; the gas can flow through porous medium and flow out. Suppose that a solid porous substance consists of combustible and inert components, and at the same time the solid combustible material transforms into a gas in the reaction with gaseous oxidizer, so we have the following expression:

$$\text{Solid Fuel} + (\mu)\text{Oxidizer} \rightarrow (1 + \mu)\text{Gaseous Product},$$

where $\mu$ is the mass stoichiometric coefficient for oxidizer.

The model is based on the assumption of interacting interpenetrating continua [14] using the classical approaches of the theory of filtration combustion [1]–[3]. In the energy equation for the solid components not only heat generation is taken into account but also the thermal conductivity and the intensity of the interphase heat exchange which is assumed to be proportional to the difference of the phase temperatures at the considered point of the medium. In the energy equation for gas the thermal conductivity is not considered because of its smallness, and it is assumed that homogeneous reactions do not occur. For describing the dynamics of gas, the equation of momentum conservation for porous media is used, which is more correct than the classical Darcy’s equation. The solid phase is assumed to be fixed, so the equation of motion for it degenerates. In the model the changes in volume and weight of the phases at their interaction are taken into account. Supposing that the diffusion of the oxidizer takes place, the perfect gas equation of state is valid. Combustion processes are described by one-step chemical reaction of
first order with respect to both arguments (the mass concentration of oxidizer and the degree of conversion of the solid combustible component). As it was shown in [15], the allowance for the temperature dependence of gas viscosity in its motion through a porous heat-evolutional medium can change the solution both quantitatively and qualitatively, so we will assume that the dynamical viscosity of gas is determined by Sutherland’s formula. Thus, the system of equations modeling the time-dependent gas flow in a porous object with zones of heterogeneous combustion is the following:

\[
\begin{align*}
(\rho_{c, f} c_{c, f} + \rho_{c, i} c_{c, i}) \frac{\partial T_c}{\partial t} = -\alpha (T_c - T_g) + Q \rho_{c, f, 0} W + (1 - a_g) \lambda_c \Delta T_c , \\
\rho_g c_{g, p} \frac{\partial T_g}{\partial t} + (\mathbf{v}_g \cdot \nabla) T_g = \alpha (T_c - T_g) , \\
\rho_g (1 + \chi (1 - a_g)) (\frac{\partial \mathbf{v}_g}{\partial t} + (\mathbf{v}_g \cdot \nabla) \mathbf{v}_g) = -a_g \nabla p + \rho_g g - a_g \frac{\mu_1}{k_1} \mathbf{v}_g - \rho_{c, f, 0} W \mathbf{v}_g , \\
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{v}_g) = \rho_{c, f, 0} W , \\
\rho_g \frac{\partial C}{\partial t} + (\mathbf{v}_g \cdot \nabla) C = \nabla \cdot (\rho_g D_g \nabla C) - \mu \rho_{c, f, 0} W - \rho_{c, f, 0} W C , \\
D_g = D_g (T_g / 273)^b , \\
\frac{\partial \eta}{\partial t} = W , \\
\rho_{c, f} = (1 - \eta) \rho_{c, f, 0} , \\
a_g = a_{g, 0} + a_{c, f, 0} \eta , \\
\mu_1 = c_{s, 1} T_g^{1.5} / (c_{s, 2} + T_g)
\end{align*}
\]

where \( a \) is the volume concentration, \( b \) is the exponent in the expression for the diffusion coefficient, \( C \) is the mass concentration of oxidizer, \( c \) is the specific heat, \( c_{s, 1} \) and \( c_{s, 2} \) are the constants in Sutherland’s formula, \( D_g \) is the diffusion coefficient of gas, \( E \) is the activation energy, \( g \) is the gravity acceleration, \( k \) is the pre-exponential factor in the expression for the rate of reaction, \( k_1 \) is the permeability coefficient, \( M \) is the molar mass of gas, \( p \) is the gas pressure, \( Q \) is the heat of reaction, \( R \) is the universal gas constant, \( t \) is the time, \( T \) is the temperature, \( \mathbf{v}_g \) is the gas velocity, \( W \) is the rate of the chemical reaction, \( \alpha \) is the constant determining the interphase heat transfer intensity, \( \eta \) is the degree of conversion of the combustible component of the solid medium, \( \lambda \) is the thermal conductivity, \( \mu_1 \) is the dynamic viscosity of the gas, \( \rho \) is the effective density, \( \chi \) is the coefficient, taking into account the inertial interaction of the phases in their relative motion [14]; subscripts: “0” denotes the initial moment, “c” denotes the condensed phase (solid medium), “i” denotes the inert component, “f” denotes the combustible component, “g” denotes the gas, “p” denotes values at constant pressure.

We assume that at the inlet of the porous object (at the lower open boundary where gas flows into the porous object) the gas pressure, the gas temperature and the mass concentration for the oxidizer are known. At the outlet (the upper open boundary where gas flows out the porous object) the pressure is known. The conditions of heat exchange at the inlet and outlet from the porous object and on the bounding impermeable walls are also known. A distinctive feature of the considered model is that the flow rate and gas velocity at the inlet to the porous object are unknown and have to be found from the solution of the problem. Thus, the boundary conditions for system (2) are as follows:

\[
\begin{align*}
p|_{x \in G_1} = p_0 (x) , \quad \lambda \frac{\partial T_c}{\partial n}|_{x \in G_1} = \beta (T_{g, 0} - T_c |_{x \in G_1}) , \\
T_g |_{x \in G_1} = T_{g, 0} \quad \text{and} \quad C |_{x \in G_1} = C_0 \quad \text{if} \quad \mathbf{v}_g |_{x \in G_1} \cdot \mathbf{n} |_{x \in G_1} > 0 , \\
\frac{\partial T_g}{\partial n}|_{x \in G_1} = 0 \quad \text{and} \quad \frac{\partial C}{\partial n}|_{x \in G_1} = 0 \quad \text{if} \quad \mathbf{v}_g |_{x \in G_1} \cdot \mathbf{n} |_{x \in G_1} > 0 ,
\end{align*}
\]
\[ \partial T_g / \partial n|_{x \in G_2} = 0, \quad \partial T_s / \partial n|_{x \in G_2} = 0, \quad \mathbf{v}_g|_{x \in G_2} \cdot \mathbf{n}|_{x \in G_2} = 0, \]

where \( G_1 \) is the object boundary opened to the atmosphere, \( G_2 \) is the impermeable boundary of the object, \( \mathbf{n} \) is the outward vector directed normally to \( G_1 \) or to \( G_2 \), \( \beta \) is the heat removal coefficient.

The permeability coefficient \( k_1 \) is usually assumed to be constant when modeling the filtration combustion in porous media. It is possible for the permeability of the combustion products to be equal to that of the initial porous substance, since permeability is determined by both the porosity and the structure of the porous medium. But typically, the combustion products are more permeable than the initial porous substance.

One of the earliest expressions for the dependence of permeability on porosity, called Kozeny equation, was proposed in [16]. A similar, but more detailed expression, called Ergun equation, was proposed in [17]. Using the Kozeny equation or neglecting the second-order term in the Ergun equation, we can write the following expression:

\[ k_1 = k_{11} \frac{a_g^3}{(1 - a_g)^2}, \]  

where \( k_{11} \) is a constant. The Kozeny (or Kozeny-Carman) equation and the Ergun equation are widely used in filtration theory. But the following expression proposed in [18] have also been used in studying of some porous media:

\[ k_1 = k_{10} \left( \frac{a_g}{a_{g0}} \right)^n, \]  

where \( n \) is usually equal to 10.

In the present work we solve system (2) using equations (4) and (5) and compare the results with the case when the permeability coefficient is constant: \( k_1 = k_{00} \). This investigation is carried out numerically by means of original computational algorithm which was proposed previously in [11] and is based on a combination of explicit and implicit finite-difference schemes. The details of the algorithm were described in [12]. It should be noted that used original algorithm is the development of another computational algorithm, which had previously been successfully used for the calculation of gas flows through porous objects with heat zones when pressure difference at the inlet and the outlet from the object is known [19]–[22].

3. Numerical investigation of 1D heterogeneous combustion taking into account the dependence of permeability on porosity

Consider the one-dimensional process of natural convection in vertical porous object, i.e. when the gas pressure at the object boundary opened to the atmosphere (at the top and at the bottom of porous object) is equal to the atmospheric pressure at assigned heights. Suppose that prior to the start time the gas flow in the object is absent and its temperature is equal to the ambient temperature \( T_{g0} \). At initial time in the place of ignition, which is located either on the object bottom or on its top, the temperature of the solid phase reaches a value \( T_{s0} \). Suppose that prior to the start time the gas flow in the object is absent and its temperature is equal to the ambient temperature \( T_{g0} \). At initial time in the place of ignition, which is located either on the object bottom or on its top, the temperature of the solid phase reaches a value \( T_{s0} \). The temperature of the solid phase exceeds the self-ignition temperature \( T_{kr} \), and burning is started. System (2) with boundary conditions (3) is solved in dimensionless variables which are introduced as follows: \( \tilde{x} = x/H, \ \tilde{t} = t/t_s, \ \tilde{v}_g = v_g/v_s, \ \tilde{p} = p/p_s, \ \tilde{\rho}_g = \rho_g/\rho_s, \ \tilde{T}_s = T_s/T_s, \ \tilde{T}_g = T_g/T_s, \ \tilde{\rho}_f = \rho_f/\rho_{f0}, \ \tilde{W} = W/W, \ \tilde{D}_g = (T_s/273)^{-b}D_g/D_{g0}; \) where subscript \( \sim \) denotes typical values or values at “normal” conditions; further in the text the tildes are removed.

In the calculations, unless otherwise stated, we use the following parameter values:

\[ H = 10 \, \text{m}, \quad t_s = 3600 \, \text{s}, \quad v_s = 1 \, \text{m/s}, \quad T_s = 300 \, \text{K}, \quad p_s = 10^5 \, \text{Pa}, \quad \rho_s = 1.2 \, \text{kg/m}^3, \]
\[ \rho_{c0} = 1.1 \cdot 10^2 \text{kg/m}^3, \quad \rho_{ci} = 6.6 \cdot 10^2 \text{kg/m}^3, \quad c_{sf} = 1.84 \cdot 10^3 J/(\text{kg} \text{K}), \]
\[ c_{ci} = 1.84 \cdot 10^3 J/(\text{kg} \text{K}), \quad \alpha = 10^3 J/(\text{m}^3 \text{K} \text{s}), \quad c_{sp} = 10^3 J/(\text{kg} \text{K}), \quad k_{00} = 10^{-8} \text{m}^2, \]
\[ c_{s1} = 1.458 \cdot 10^{-6} \text{kg/(m s K}^{1/2}), \quad c_{s2} = 110.4 \text{K}, \quad g = 9.8 \text{m/s}^2, \quad \lambda_c = 1.2 J/(\text{m} \text{K} \text{s}), \quad \beta = 10 J/(\text{m}^2 \text{K} \text{s}), \quad R = 8.31441 J/(\text{mole} \text{K}), \quad M = 2.993 \cdot 10^2 \text{kg/mole,} \quad Q = 8 \cdot 10^6 J/\text{kg}, \]
\[ k = 3.16 \cdot 10^7 \text{/s} \quad [23], \quad E = 110 \cdot 10^3 J/\text{mole} \quad [23], \quad D_{g0} = 1.82 \cdot 10^{-5} \text{m}^2/\text{s}, \]
\[ b = 1.724, \quad \mu = 2.667, \quad a_{g0} = 0.3, \quad a_{c0} = 0.1, \quad \chi = 0.5, \]

and the dimensionless boundary conditions:
\[ T_{g0} = 1 \quad \text{and} \quad C_0 = 0.23. \quad (7) \]

We select the coefficients \( k_{11} \) and \( k_{10} \) so that the initial permeability \( k_1 \) in these cases is equal to the constant permeability \( k_{00} = 10^{-8} \text{m}^2 \), which is also used for solving system (2).

We also assume that if the temperature of the solid medium below the temperature of self-ignition \( T_{kr} = 1.1 \), the exothermic reactions do not occur.

At first we consider the case when the ignition zone is located at the bottom of the porous object. For arising self-sustaining cocurrent combustion wave, the changing of permeability due to the changing of porosity does not lead to the temperature increasing in the combustion zone, but leads to the speed increasing of the combustion wave. This fact is clearly demonstrated in Fig. 1, which shows the distribution of solid medium temperature in the considered porous object at \( t = 700 \) at different permeability coefficient when the width of ignition zone located at the bottom of the object is equal to 1/10 and the initial ignition temperature \( T_{c0} \) is equal to 2.5.

**Figure 1.** Distribution of the solid medium temperature in the porous object at \( t = 700 \) at different permeability coefficient when the width of ignition zone located at the bottom of the object is equal to 1/10 and the initial ignition temperature \( T_{c0} \) is equal to 2.5.

Combustion changes porosity, and if the permeability depends on porosity, the resistance of the porous medium decreases and gas velocity increases; this leads to increasing of the
oxidizer supply, so the combustion wave propagates with a higher speed. Note that when we use equation (5) the permeability is modified more than when using equation (4). At the same time, when we use $n$ equal to 10 in equation (5), the permeability is modified more than when using $n$ equal to 8 in this equation. Thus, as can be seen from the Fig. 1, the more changes in permeability due to changes in porosity, the greater the speed of the combustion wave increases.

Consider the case when the ignition zone is located at the top of the porous object. For arising self-sustaining countercurrent combustion wave, the changing of permeability due to the changing of porosity leads to increasing both the temperature in the combustion zone and the speed of the combustion wave. This fact is clearly demonstrated in Fig. 2, which shows the distribution of solid medium temperature in considered porous object at $t = 850$ at different values of the permeability coefficient when the width of ignition zone located at the top of the object is equal to $1/10$ and the initial ignition temperature $T_{c0}$ is equal to 2.5 for the “direct” wave propagation, i.e. when combustion wave moves down.

![Figure 2. Distribution of the solid medium temperature in the porous object at $t = 850$ at different values of the permeability coefficient when the width of ignition zone located at the top of the object is equal to $1/10$ and the initial ignition temperature $T_{c0}$ is equal to 2.5 for “direct” wave propagation.](image)

As for the countercurrent combustion wave, the rate of oxygen supply controls the process, increasing gas velocity due to decreasing resistance of the porous medium leads to increasing degree of conversion of the solid combustible component, so the temperature in the combustion zone increases with time. And the more changes in permeability due to changes in porosity, the greater the temperature and the speed of the combustion wave increase.

When the countercurrent combustion wave reaches the lower boundary of the object, it is reflected and starts to move up with reburning completely the remaining solid combustible substance. This reflected wave is cocurrent wave, so the propagation of the reflected wave is similar to the propagation of the cocurrent combustion wave which was considered earlier. Thus, in this case the changing of permeability due to the changing of porosity does not lead to the temperature increasing in the combustion zone, but leads to a significant speed increasing of the combustion wave. This fact is clearly demonstrated in Fig. 3, which shows the distribution of
solid medium temperature in considered porous object at different times at different values of the permeability coefficient when the width of ignition zone located at the top of the object is equal to 1/10 and initial ignition temperature $T_{c0}$ is equal to 2.5 for “reflected” wave propagation, i.e. when combustion wave moves up after the reflection from the bottom.

**Figure 3.** Distribution of the solid medium temperature in the porous object at different times at different values of the permeability coefficient when the width of ignition zone located at the top of the object is equal to 1/10 and the initial ignition temperature $T_{c0}$ is equal to 2.5 for “reflected” wave propagation.

We can see again, that the more changes in permeability due to changes in porosity, the greater the speed of the combustion wave increases. It should be noted that the small temperature oscillation can be seen in the high-temperature zone of cocurrent combustion wave. When the temperature in cocurrent combustion wave is sufficiently high, oscillatory instabilities may occur for both constant and variable permeabilities, which is typical for kinetically controlled processes, but it is not discussed in this paper.

Thus, the considered dependence of permeability on porosity, which is described by equations (4) or (5), leads mainly to quantitative changes in solution of the system of equations (2) in one-dimensional case. Qualitative change is the increase of the temperature in the combustion zone with time in the countercurrent wave.

4. Conclusions
The one-dimensional unsteady process of heterogeneous combustion in porous object under free convection is considered when the dependence of permeability on porosity is taken into account. Using original computational algorithm, numerical investigations are carried out with some known equations which describe the changing of permeability due to the changing of porosity. It is shown that for both cocurrent and countercurrent self-sustaining combustion waves the changing of permeability due to the changing of porosity leads to the speed increasing of the combustion wave. For self-sustaining countercurrent combustion wave the changing of permeability due to the changing of porosity can also increase the temperature in the combustion zone with time.
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