Multidimensional computational models of gas combustion in heterogeneous porous medium

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Abstract. The processes of filtration gas combustion in heterogeneous porous medium is studying. The presence of two opposite modes of front propagation made it possible to stabilize the combustion front in a composite porous medium with piecewise constant porosity. A feature of this study is the presentation of the original model not in the traditional form of a system of parabolic equations, but in the form of integral conservation laws in terms of the temperature of the porous medium, the total gas enthalpy, and the mass of gas mixture, and the fluxes corresponding to these functions.

1. Introduction
The process of the filtration gas combustion (FGC) front propagation was first experimentally and theoretically studied in [1, 2]. A definition of the FGC, revealing the essence of this phenomenon, was given in [3]: “Filtration gas combustion may be defined as the propagation of region of gaseous exothermic reaction in chemically inert porous medium, as the gaseous reactants seep into the region of chemical transformation”. These papers show the possibility of the combustion front propagation both in the direction of the gas flow and upstream. At the same time, it was experimentally established in [4] that when the direction of front propagation changes from upstream to downstream movement, stability is lost, and the combustion front disintegrates. This paper shows how the presence of two such modes of propagation of the combustion front allows the front to be stabilized. An inhomogeneous porous medium consisting of two parts with different thermophysical characteristics is considered. Let us note that in all the models under consideration here, we speak about the slow propagation of the front, and the values of the flow rate of the gas mixture make it possible to neglect the pressure change in the system, which is one of the main characteristics of the filtration process. In this sense, the slow FGC process we are considering can be characterized as “filtration without filtration”.

In [5, 6] two-temperature computational models of the FGC are proposed in the form of a system of conservation laws represented by a system of first-order equations. The numerical implementation of these models is based on spatial approximation by the mixed finite element method [9] and the method of fractional time steps for multidimensional problems [10]. In distinguish from [5, 6] in this paper we investigated the process FGC in inhomogeneous porous media in the case of a jump of a porosity. The computational FGC models in the form of a system of grid parabolic equations were considered in [7, 8]. In these papers the possibility of combustion stabilization was established.
2. Conservation laws in heterogeneous porous medium

The FGC process can be described by the following physical model: a combustible gas mixture enters the elongated parallelepipedal domain $\Omega$ filled with a chemically inert porous medium at a rate of $v$, and after the initiation of combustion, a moving front appears that separates the zone of the fresh mixture from zone of combustion products and moving either against the flow or in the direction of the gas flow. The basis of mathematical model is the energy conservation laws for the temperature of the porous medium ($T_s$) and the gas ($T_g$), and the mass conservation law for the relative concentration of the reacting component of the gas mixture $\eta$. In this case, the homogenization of the model is carried out on the basis of a two-temperature approach, when at each point of a continuous medium, a solid and a gas phase with Newtonian (linear) heat transfer between them are specified.

Below the following notations will be used: $\phi$ is porosity, $D$ is diffusion coefficient, $\rho_i$, $c_i$, $\lambda_i$ are density, specific heat at constant pressure and thermal conductivity coefficient of the $i$-th phase, where $i = s$ and $i = g$ correspond to the the porous media and to the gas mixture, $v$ is the gas velocity vector, $\alpha$ is the intensity of interphase heat transfer, $Q$ is the thermal effect of the chemical reaction. Formulation of the conservation law for the gas mixture will use, so called, relative full gas enthalpy $H$ instead of the gas temperature $T_g$:

$$H = T_g + \frac{Q}{c_g} \eta.$$  \hspace{1cm} (1)

In the computational model, it is preferable to use the function $H$, since then a balance is automatically ensured between the release of energy due to a chemical reaction and the consumption of the combustion mixture. The model considers the first-order reaction with heat release according to the Arrhenius law:

$$W(\eta, H) = \eta Z(\eta, H), \quad Z(\eta, H) = k_0 \exp \left( -\frac{E}{R(H - Q\eta/c_g)} \right).$$  \hspace{1cm} (2)

where $E$, $R$ and $k_0$ are the activation energy, the universal gas constant, and the preexponent characterizing the rate of a chemical reaction. In what follows, it will be assumed that the similarity of concentration and temperature fields holds, which is expressed in the equality of the diffusion coefficients and thermal diffusivity of the gas:

$$D = \frac{\lambda_g}{c_g \rho_g}$$  \hspace{1cm} (3)

(see, for example, [11]). Some other details may be found in [6].

Below we will use the notation $\theta = T_s - T_0$, where $T_0$ is a temperature of "cold" gas. In accordance with (1), (3) conservation laws may be written in the form:

$$\left(1 - \phi\right)c_s \rho_s \frac{\partial \theta}{\partial t} + \nabla \cdot w_\theta = \alpha (H - \theta - \frac{Q}{c_g} \eta - T_0),$$  \hspace{1cm} (4)

$$\phi c_g \rho_g \frac{\partial H}{\partial t} + \nabla \cdot w_H - \frac{c_g \rho_g}{\lambda_g} \alpha \nabla \cdot w_H = \alpha (\theta - H + \frac{Q}{c_g} \eta + T_0),$$  \hspace{1cm} (5)

$$\phi \rho_g \frac{\partial \eta}{\partial t} + \nabla \cdot w_\eta - \frac{1}{D} \nabla \cdot w_\eta = -\phi \rho_g \eta Z(\eta, H),$$  \hspace{1cm} (6)

where the flux of the heat in porous media, the flux of the relative gas enthalpy and the flux of the concentration of gas mixture are defined as follows:

$$w_\theta = -(1 - \phi) \lambda_s \nabla \theta, \quad w_H = -\phi \lambda_g \nabla H, \quad w_\eta = -\phi \rho_g D \nabla \eta,$$  \hspace{1cm} (7)
For the reduced system of equations, let us set the boundary conditions. Let the problem be considered in the domain
\[ \Omega = (0, L_x) \times (0, L_y) \times (0, L_z). \]
On the left boundary \((x = 0)\) the Dirichlet conditions are set:
\[ \theta = 0, \quad H = T_b, \quad \eta = 1. \] (8)
Here and further \(T_b = T_0 + Q/c_g\) is the adiabatic combustion temperature \([11]\). On the other sides of \(\partial \Omega\) the Neumann conditions are set:
\[
\mathbf{w}_\theta \cdot \mathbf{n} = \beta \theta, \quad \mathbf{w}_H \cdot \mathbf{n} = 0, \quad \mathbf{w}_\eta \cdot \mathbf{n} = 0, \quad (9)
\]
where \(\mathbf{n}\) is the unit vector of outer normal to the boundary of the domain \(\Omega\), and \(\beta = 0\) at \(x = L_x\). Conditions (9) mean that heat loss occurs only from the porous media on the lateral sides \(\partial \Omega \setminus \{x = 0, x = L_x\}\).

Let us note that equations (4)-(7) are valid in subdomains, where the porosity \(\phi\) is smooth function. But the problem of our interest includes the case of discontinuous function \(\phi\). In this connection, we turn to a generalized formulation of the problem, in which, from some integral identities, the functions \(\theta, H, \eta, \) and the corresponding flows are defined simultaneously. In this case, the functions \(\theta, H, \eta\) can be discontinuous, and the corresponding flows have square-summable components and divergence. Omitting well-known details (see, for example, \([9]\)), we write down the corresponding system of integral identities that hold for any square-summable scalar function \(\chi\) and for any vector-function \(\mathbf{u}\) with square-summable components and divergence, and \( \mathbf{u} \cdot \mathbf{n} = 0 \) on \(\partial \Omega \setminus \{x = 0\}\).

\[
\int_\Omega (1 - \phi) c_s \rho_s \frac{\partial \theta}{\partial t} \chi \, dx + \int_\Omega (\nabla \cdot \mathbf{w}_\theta + \boldsymbol{\alpha}(\theta - H + \frac{Q}{c_g}\eta)) \chi \, dx = -T_0 \int_\Omega \chi \, dx,
\]
\[
\int_\Omega \frac{1}{(1 - \phi) \lambda_g} \mathbf{w}_\theta \cdot \mathbf{u} \, dx - \int_\Omega \theta \nabla \cdot \mathbf{u} \, dx + \int_{\partial \Omega \setminus \{x = 0\}} \frac{1}{\beta} (\mathbf{w}_\theta \cdot \mathbf{n}) (\mathbf{u} \cdot \mathbf{n}) \, d\gamma = 0,
\]
(10)
\[
\int_\Omega \phi c_g \rho_g \frac{\partial H}{\partial t} \chi \, dx + \left( \nabla \cdot \mathbf{w}_H - \frac{c_g \rho_g}{\lambda_g} \mathbf{v} \cdot \mathbf{w}_H + \boldsymbol{\alpha}(H - \theta - \frac{Q}{c_g}\eta) \right) \chi \, dx = T_0 \int_\Omega \alpha \chi \, dx,
\]
\[
\int_\Omega \frac{1}{\phi \lambda_g} \mathbf{w}_H \cdot \mathbf{u} \, dx - \int_\Omega H \nabla \cdot \mathbf{u} \, dx = -T_b \int_{\{x = 0\}} \mathbf{u} \cdot \mathbf{n} \, d\gamma,
\]
(11)
\[
\int_\Omega \phi \rho_g \frac{\partial \eta}{\partial t} \chi \, dx + \int_\Omega \chi \nabla \cdot \mathbf{w}_\eta \, dx - \int_\Omega \frac{1}{D} \mathbf{v} \cdot \mathbf{w}_\eta \chi \, dx + \int_\Omega \phi \rho_g \eta \mathbf{Z}(\eta, H) \, dx = 0,
\]
\[
\int_\Omega \frac{1}{\phi \rho_g D} \mathbf{w}_\eta \cdot \mathbf{u} \, dx - \int_\Omega \eta \nabla \cdot \mathbf{u} \, dx = - \int_{\{x = 0\}} \mathbf{u} \cdot \mathbf{n} \, d\gamma,
\]
(12)
In deriving these equalities the boundary conditions (8), (9) were used essentially. In the terminology \([9]\), used in mixed formulations of the type (10)-(12), equalities (8) and the first equality from (9) are "the natural boundary conditions" that directly enter into the above integral identities. "The main boundary conditions" are the second and the third conditions from (9). A solution and an arbitrary vector function \(\mathbf{u}\) must satisfy a priori to these conditions. Let us note that if \(\beta \to \infty\) then according to (9) \(\theta = 0\), and the last term in (10) disappears. If \(\beta \to 0\) then \(\mathbf{w}_\theta \cdot \mathbf{n} = 0\), and the first condition from (9) becomes the main boundary condition.
3. Numerical algorithm for 3D problem

The spatial approximation of the problem (10)-(12) is carried out by the mixed finite element method on a rectangular uniform grid using the Raviart-Thomas elements (see [9]). As a result the following system of ordinary differential equations for grid functions we obtain:

\[
\begin{align*}
C_\theta \frac{d\theta}{dt} + B_\theta^I w_\theta + C_\alpha \left( \theta - H + \frac{Q}{c_g} \eta \right) &= -T_0 F_\alpha, & A_\theta w_\theta - B_\theta \theta &= 0, \\
C_H \frac{dH}{dt} + B_H^I w_H + C_\alpha \left( H - T - \frac{Q}{c_g} \eta \right) &= T_0 F_\alpha, & A_H w_H - B_H H &= T_1 F_H, \\
C_\eta \frac{\partial \eta}{\partial t} + B_\eta^I w_\eta + C_\eta \eta Z(\eta, H) &= 0, & A_\eta w_\eta - B_\eta \eta &= F_\eta.
\end{align*}
\]

We use the same notations for grid functions as for the functions from previous section. Mass matrices $C_\theta$, $C_H$, $C_\eta$, and $C_\alpha$ are diagonal, $A_\theta$, $A_H$, and $A_\eta$ are block-diagonal with tree-diagonal blocks,

\[
B_\theta = \begin{pmatrix} (B_\theta)_x \\ (B_\theta)_y \\ (B_\theta)_z \end{pmatrix}, \quad B_H = \begin{pmatrix} (B_H)_x \\ (B_H)_y \\ (B_H)_z \end{pmatrix}, \quad B_\eta = \begin{pmatrix} (B_\eta)_x \\ (B_\eta)_y \\ (B_\eta)_z \end{pmatrix},
\]

where the usage the upwinding gives two-diagonal matrices $(B_i)_x$, $(B_i)_y$, $(B_i)_z$, $i = \theta, H, \eta$ with diagonal dominance.

An approximation of system (13) in time is carried out by a splitting scheme like the fractional steps method [10]. Similar to [6], we present the splitting scheme in the form of the following step-by-step algorithm:

\[
\begin{align*}
C_\eta \eta^{n+\frac{1}{2}} + \tau (B_\eta)_z^I (w_\eta)_z^{n+\frac{1}{2}} &= C_\eta \eta^n, & (A_\eta)_z^I (w_\eta)_z^{n+\frac{1}{2}} - (B_\eta)_z \eta^{n+\frac{1}{2}} &= (F_\eta)_z; \\
C_\eta \eta^{n+\frac{1}{2}} + \tau (B_\eta)_y^I (w_\eta)_y^{n+\frac{1}{2}} &= C_\eta \eta^n, & (A_\eta)_y^I (w_\eta)_y^{n+\frac{1}{2}} - (B_\eta)_y \eta^{n+\frac{1}{2}} &= (F_\eta)_y; \\
[1 + \tau Z(\eta^n, H^n)] C_\eta \eta^{n+1} + \tau (B_\eta)_x^I (w_\eta)_x^{n+1} &= C_\eta \eta^{n+\frac{1}{2}}, & (A_\eta)_x^I (w_\eta)_x^{n+1} - (B_\eta)_x \eta^{n+1} &= (F_\eta)_x; \\
C_H H^{n+\frac{1}{2}} + \tau (B_H)_z^I (w_H)_z^{n+\frac{1}{2}} &= C_H H^n, & (A_H)_z^I (w_H)_z^{n+\frac{1}{2}} - (B_H)_z H^{n+\frac{1}{2}} &= T_b (F_H)_z; \\
C_\theta \theta^{n+\frac{1}{2}} + \tau (B_\theta)_z^I (w_\theta)_z^{n+\frac{1}{2}} &= C_\theta \theta^n, & (A_\theta)_z^I (w_\theta)_z^{n+\frac{1}{2}} - (B_\theta)_z \theta^{n+\frac{1}{2}} &= 0; \\
C_H H^{n+\frac{1}{2}} + \tau (B_H)_y^I (w_H)_y^{n+\frac{1}{2}} &= C_H H^n, & (A_H)_y^I (w_H)_y^{n+\frac{1}{2}} - (B_H)_y H^{n+\frac{1}{2}} &= T_b (F_H)_y; \\
C_\theta \theta^{n+\frac{1}{2}} + \tau (B_\theta)_y^I (w_\theta)_y^{n+\frac{1}{2}} &= C_\theta \theta^n, & (A_\theta)_y^I (w_\theta)_y^{n+\frac{1}{2}} - (B_\theta)_y \theta^{n+\frac{1}{2}} &= 0; \\
C_H + \tau C_\alpha H^{n+1} + \tau (B_H)_x^I (w_H)_x^{n+1} &= C_H H^{n+\frac{1}{2}} + \tau C_\alpha \left( \theta^{n+\frac{1}{2}} + \frac{Q}{c_g} \eta^{n+1} + T_0 F_\alpha \right), & (A_H)_x^I (w_H)_x^{n+1} - (B_H)_x H^{n+1} &= T_b (F_H)_x; \\
(C_\theta + \tau C_\alpha) \theta^{n+1} + \tau (B_\theta)_x^I (w_\theta)_x^{n+1} &= C_\theta \theta^{n+\frac{1}{2}} + \tau C_\alpha \left( H^{n+1} - \frac{Q}{c_g} \eta^{n+1} - T_0 F_\alpha \right), & (A_\theta)_x^I (w_\theta)_x^{n+1} - (B_\theta)_x \theta^{n+1} &= T_b (F_\theta)_x.
\end{align*}
\]

In [6] efficient algorithm of implementation of each step of this splitting scheme is presented. In the case of constant porosity and in the absence of heat loss ($\phi = \text{const}$, $\beta = 0$), the problem actually becomes one-dimensional, and at $-\infty < x < \infty$ the solution is invariant with respect to the transformation $\xi = x - ut$, where $u$ is the constant propagation velocity of combustion front. Moreover, as noted in [12], the following equality holds:

\[
u = \frac{H_c - T_b}{H_c - T_b + \sigma \theta_x} v, \quad \sigma = \frac{(1 - \phi)c_s \rho}{\phi c_g \rho_g} \tag{15}
\]
where \( \theta_c = \theta(\infty) \) and \( H_e = H(\infty) \) are the equilibrium temperature of the porous medium and the relative enthalpy. Here \( \theta \) and \( H \) are functions of variable \( \xi \). In distinguish from papers [5], [6] this article deals with discontinuous porosity. Then the solution of the problem at \(-\infty < x < \infty\) is not invariant with respect to the transformation \( \xi = x - ut \). However, in the case of piecewise constant porosity in the interval where \( \phi = \text{const} \) far from the points of discontinuity of \( \phi \), formula (15) can be applied in the interval of the functions \( \theta \) and \( H \) stabilization behind the combustion front. According to this remark we will use the equality (15) below.

4. Stabilization of combustion front

In this section, we present the results of numerical experiments for piecewise constant porosity. In this case, the parallelepiped \( \Omega \) is divided into two parallelepipeds \( \Omega^- \) and \( \Omega^+ \) corresponding to the intervals \( 0 \leq x < x_0 \) and \( x_0 \leq x \leq L_x \). Combustion is initiated in the domain \( \Omega^+ \), and the combustion front moves to the left towards the value \( x = x_0 \). In all experiment below we use the value \( \phi = \phi^+ = 0.5 \) in the subdomain \( \Omega^+ \), and \( \phi = \phi^- \) in the subdomain \( \Omega^- \) will be varied. In subsections below numerical results for the 1D and 2D problems will be demonstrated separately.

We use the following values of the physical parameters:

\[
L_x = 0.1 \text{ m}, \quad L_y = 0.02 \text{ m}, \quad D = 5 \cdot 10^{-5} \text{ m}^2/\text{s}, \quad \alpha = 10^7 \text{ W/m}^3 \cdot \text{K},
\]

\[
\rho_s = 10^3 \text{ kg/m}^3, \quad c_s = 10^3 \text{ J/kg} \cdot \text{K}, \quad \lambda_s = 2 \text{ W/m} \cdot \text{K},
\]

\[
\rho_y = 1 \text{ kg/m}^3, \quad c_y = 2 \cdot 10^3 \text{ J/kg} \cdot \text{K}, \quad \lambda_y = 0.1 \text{ W/m} \cdot \text{K},
\]

\[
T_0 = 300 \text{ K}, \quad Q/c_g = 1100 \text{ K}, \quad k_0 = 10^{12} \text{ s}^{-1}, \quad E/R = 2 \cdot 10^4 \text{ K}.
\]

In experiments for a two-dimensional problem, we will set \( v_y = 0 \). The values of \( v_x = v \) will be varied. In addition, different values of the intensity of external heat losses \( \beta \) will be used.

4.1. Numerical results for one-dimensional problem

This subsection discusses the results of computational experiments for a one-dimensional problem. Figure 1 shows the dependences of the front velocity on the porosity in the interval \( 0 \leq x < x_0 \). In the experiment, it was assumed that \( x_0 = 0.05 \text{ m} \), and a combustion was initiated in the interval \( x_0 \leq x \leq L_x \). The following notations are used in the figures: \( u_{\text{theor}} \) is the front velocity obtained according to formula (15), and \( u_{\text{real}} \) is the front velocity obtained by direct observation of the solution to the problem. It can be seen that when approaching the critical value of porosity \( \phi_{\text{cr}} \) when stabilization occurs \( (u = 0) \), formula (15) stops working. This is quite natural, since this formula was obtained from the balance relations on the interval \( -\infty < x < \infty \) when the solution is invariant with respect to the transformation \( \xi = x - ut \). Figure 1 shows the results for two velocities \( v = 2 \text{ m/s} \) and \( v = 3 \text{ m/s} \), and the values of the critical porosity differ significantly (indicated by the dashed line).

4.2. Numerical results for two-dimensional problem

For a two-dimensional problem, the dependence of the critical porosity was established, above which the stabilization of the FGC process begins. The calculations were carried out practically without heat loss: \( \beta = 1 \text{ W/m}^2 \cdot \text{K} \). Figure 2 demonstrates the dependence of critical values of porosity \( \phi_{\text{cr}} \) on gas mixture velocity. The resulting curve is close to the straight line \( \phi_{\text{cr}} = 1.126 - 0.156 \nu \). Those, the stabilization area is above this line, or approximately \( u = 0 \) at \( \phi^- \geq 1.126 - 0.156 \nu \).

Figure 3 shows the results of the experiment in the two-dimensional case, demonstrating the stabilization process itself: after the 15th second of physical time, the temperature of the porous medium stops changing. Note that not only the position of the front is stabilized, but also its shape. The calculations were carried out at \( \beta = 10^3 \text{ W/m}^2 \cdot \text{K} \).
Let us note that the presence of heat loss can lead to combustion instability up to the extinguishing of the flame. In this case, the occurrence of instability is influenced not only by the intensity of heat loss $\beta$, but also at what flow rate the heat loss is realized. The corresponding illustration is demonstrated by figure 4. The figure shows the temperatures of the porous medium at the time moment $t = 16$ s at the same intensity of heat loss $\beta = 10^3$ W/m$^2$·K, but at different gas flow rates: $v = 3$ m/s for option (a) and $v = 1$ m/s for option (b). With such heat losses at a gas flow rate corresponding to the velocity $v = 1$ m/s, the fresh gas mixture is not enough to maintain a stable motion of the combustion front.

5. Conclusion
A three-dimensional computational model of filtration gas combustion in a porous medium with piecewise constant porosity has been constructed. The model is based on a system of integral energy and mass conservation laws. The numerical implementation of the model uses a mixed finite element method of spatial approximation in combination with the method of fractional steps on time approximation.

As a result of the research, a simple mechanism of stabilization of the front of filtration gas combustion is described. The essence of this mechanism is the implementation of the process in

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**Figure 1.** Dependence of front velocity on porosity in the left subdomain:

(a) $v = 2$ m/s, (b) $v = 3$ m/s.

**Figure 2.** Dependence of critical porosity on gas velocity.
a composite porous medium with different thermophysical characteristics. In this study, variable porosity was considered. The stabilization mechanism is based on the selection of thermophysical characteristics in such a way that the combustion front, being initiated in each subdomain with constant characteristics, moves towards the discontinuity of the parameters.

**Acknowledgments**

This work was supported by the Russian Science Foundation (grant 19-11-00048).
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