Gas heat exchange at inhomogeneous combustion of solid porous media

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Abstract. The authors suggest using a numerical method based upon the finite element analysis of the equations of continuous inhomogeneous media mechanics to describe thermophysical properties of transient motions of viscous gas through porous media with chemical changes and phase transitions in a solid phase. The model takes into account heat exchange between a solid frame and gas, changes in the phase volume and mass at interaction, the presence of oxidant diffusion. The software developed in FreeFem++ allows clear and vivid studying the process of gas combustion in solid porous medium with inhomogeneous combustion source at forced filtration in the course of time as well as modeling and analyzing a real experiment.

1. Introduction

Filtration gas combustion processes are widely applied in everyday routine and chemical technology. Peat fire, cigarette smoking can be modeled as the combustion of solid porous media.

The article relevance is explained by the fact that the process of porous rock inhomogeneous combustion is inseparable associated with various catastrophes both technogenic and natural. Such catastrophes can include combustion occurrence at fire explosive facilities, peat bogs and waste deposits. The study of motion structure and gas heat exchange at the combustion of solid porous rocks helps to develop understanding of the nature of these processes. This will facilitate the prevention of fires or their extinguishing.

The numerical analysis of two-dimensional gas fluids in porous media with inhomogeneous combustion sources at forced filtration and free convection was conducted in the papers \cite{1, 2} developing a numerical method based upon the combination of explicit and implicit finite-difference schemes. According to the proposed method, the equations of power, impulse conservation and oxidant concentration are transformed into explicit finite-difference equations while the continuity equation is transformed into an implicit finite-difference equation. Further research were developed in the area of modeling gas motion through the layer of a heat accumulating material with phase transition \cite{3}. In \cite{4} – \cite{6} analyzed the research of smoldering in foamed polyurethane at free convection.

The authors study a stationary porous object having lateral walls which are impenetrable and thermally non-conductive and open on the top and bottom. Cold gas can flow into a porous object and flow out through open boundaries. A solid porous substance consists of a combustible component,
inert additive and solid reaction products when a solid combustible material is transformed into gas and solid products of the reaction as a result of interaction with a gaseous oxidant.

At the research of filtration gas combustion it is possible to use a volume-averaged model [7], i.e. one can use efficient (averaged in terms of volume) thermophysical properties of a porous frame and gas while cross-media interaction is described by the heat exchange factor.

A mathematical model is built upon the equations of thermal balance in solid and gaseous phases, mass transfer of gas components, continuity equations, the equations of diffusion hydrodynamics or gas filtration and state [8]. To form source terms of the equations of thermal balance and mass, the authors set down chemical kinetics equations of the considered gas components [9], [7] and state boundary conditions.

A system of differential equations, describing the thermal conductive gas dynamics in porous medium, is a linear mixed hyperbolic-parabolic equation system. In addition, to close the system one can use equations in ordinary derivatives.

In a general case this problem cannot be resolved analytically. The paper suggests a new calculation algorithm in the integrated development software FreeFem++ [10] implemented on the basis of finite-dimensional analysis allowing one to study heat exchange through porous media with chemical transformations and phase transitions in the solid phase.

2. Mathematical model

The mathematical model of viscous gas thermal conductivity at the filtration combustion of solid porous bodies is considered as the motion of two-component continuous medium consisting of solid and gaseous media within the model of multispeed continuum and interpenetrating motion of the mix components [9], [7].

The system of differential equations modeling the process is based upon a mathematical model suggested in [1], [2].

A equation system used for modeling heat transfer of non-stationary gas flows in porous media with inhomogeneous combustion sources is written as follows [1], [2]:

\[
\begin{align*}
\left(\rho_{cf}c_{cf} + \rho_{ci}c_{ci} + \rho_{cp}c_{cp}\right) \frac{\partial T_c}{\partial t} &= -\alpha(T_c - T_g) + Qp_{cf0}W + \lambda_c \text{div}\left((1 - a_g)\nabla T_c\right), \\
\rho_g \left[\frac{\partial T_g}{\partial t} + \left(\nabla T_g \cdot \mathbf{v}\right)\right] &= \alpha(T_c - T_g) + \lambda_g \text{div}(a_g \nabla T_g), \\
\rho_g \left[1 + 0.5(1 - a_g)\right] \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v}\right] &= -a_g \nabla p + \rho_g \mathbf{g} - a_g \mu_k \mathbf{k}^{-1} \mathbf{v} - (1 - \mu_p)\rho_{cf0}W \mathbf{v}, \\
\frac{\partial \rho_g}{\partial t} + (\nabla \rho_g \cdot \mathbf{v}) + \rho_g \text{div} \mathbf{v} &= (1 - \mu_p)\rho_{cf0}W, \quad p = \rho_g R T_g / (a_g M), \\
\rho_g \left[\frac{\partial C}{\partial t} + (\nabla C \cdot \mathbf{v})\right] &= \text{div}\left(\rho_g D_g \nabla C\right) - \mu_g \rho_{cf0}W - (1 - \mu_g)\rho_{cf0}W C, \\
W &= (1 - \eta) C \exp[-E/(RT_c)], \\
\frac{\partial \eta}{\partial t} &= W, \quad \eta(0) = 0, \\
\rho_{cf} &= (1 - \eta)\rho_{cf0}, \quad \rho_{cp} = \mu_p \rho_{cf0} \eta, \\
a_g &= a_{g0} + (a_{cf0} - a_{cpEnd}) \eta, \\
D_g &= D_{g0}(T_g/273)^b, \quad \mu = c_{s1} T_g^{1.5} / (c_{s1} + T_g).
\end{align*}
\]

where \(T_c\) is solid medium temperature, \(T_g\) is gas temperature, \(\rho_g\) is gas density, \(C\) is oxidant mass concentration, \(W\) is chemical reaction rate, \(\eta\) is solid combustible conversion, \(a_g\) is gas volumetric concentration, \(a_{g0}\) is gas volumetric concentration at the initial instant, \(a_{cf0}\) is fuel volumetric concentration at the initial instant, \(a_{cpEnd}\) is volumetric concentration of the reaction product condensed phase at the finite time moment, \(E\) is activation energy, \(D_g\) is gas diffusion factor, \(b\) is
exponential factor in the equation for the gas diffusion factor, $\rho_{cf}$ is fuel density, $\rho_{cp}$ is reaction product density, $\nu$ gas velocity, $g$ is gravity acceleration.

At the inlet to the porous object (boundary $\Gamma_1$) the following values are known: gas temperature and pressure as well as oxidant mass concentration. At the outlet of the object (boundary $\Gamma_2$) the pressure is known. Additionally, the authors set the heat exchange conditions at the inlet and outlet of the porous object and limiting impermeable walls (boundary $\Gamma_0$). We can write the boundary conditions for equations (1) – (9) in the following form:

\[
\begin{align*}
 p = p_0(x,y), & \quad \partial T_c/\partial n = (\beta/\lambda_c) (T_g - T_c), \quad T_g = T_{g0}, \quad C = C_0, \quad (x,y) \in \Gamma_1 \\
 & \quad \text{if } (\nu \cdot n) \leq 0, \quad (x,y) \in \Gamma_1;
\end{align*}
\]

\[
\begin{align*}
 p = p_1(x,y), & \quad \partial T_c/\partial n = (\beta/\lambda_c) (T_g - T_c), \quad \partial T_g/\partial n = 0, \quad \partial C/\partial n = 0, \quad (x,y) \in \Gamma_2 \\
 & \quad \text{if } (\nu \cdot n) > 0, \quad (x,y) \in \Gamma_2;
\end{align*}
\]

\[
\begin{align*}
 \partial T_c/\partial n = 0, & \quad \partial T_g/\partial n = 0, \quad \partial C/\partial n = 0, \quad (x,y) \in \Gamma_0, \\
 & \quad (\nu \cdot n) = 0, \quad (x,y) \in \Gamma_0,
\end{align*}
\]

where $\beta$ is the heat removal coefficient.

Boundary conditions are obtained using the following values:

\[
\begin{align*}
 T_{g0} = 1, \quad C_0 = 0.23, \quad p_0 = 1.1, \quad p_1 = 1, \quad T_c = \begin{cases} 1, & \text{in the zone without burning}, \\ 2, & \text{in the combustion zone}. \end{cases}
\end{align*}
\]

3. Numerical modelling

When modeling a system with continuous time, a system with discrete time in the power equation and in the equations of oxidant concentration and continuity applies the inverse Euler method of the first order [11] while the concentration equation is transformed with the help of the direct Euler method [11].

In this case, the thermal properties of the medium depend on the temperature, in this sense all the equations included in the system are linear. Non-linearity has a non-monotonic nature.

We will study the linearized model, which is characterized by the fact that the solution at the new temporary layer is derived from the solution of the linear differential problem, the coefficients of the derivatives are taken from the previous temporary layer, while a modified Newton method is used to linearize a non-linear term in the right part of the equation, describing the reaction oxidation [12]. In addition, the continuity equation is replaced by a more regularized equation by means of adding an elliptic component with a regularization parameter.

Note that two-dimensional gas motions at inhomogeneous combustion of solid porous media were numerically studied [1], [2]. The advantage of this method is that the selection of implicit schemes allows modeling quite a long period of combustion at minimum time expenditures for software calculation [12], [12].

It seems impossible to prove the analytical convergence of the approximated solution to exact solution. The study of the approximated solution convergence was conducted both by means of comparison with the available computational data and by the experiments with the help of grid condensation and reducing time increment. The convergence analysis of the obtained solution on two computational grids, with the number of nodes on one twice more than on the other, showed that the convergence of the solution is achieved with the number of computational nodes of approximately 13912 which corresponds to $h=0.02$.

In the case of forced filtration, when a self-sustaining combustion occurs, the reaction wave moves up and towards the side walls, completely burning the combustible substance.
Figures 1 and 2 give an example of the gas velocity field, as well as the degree of conversion of the combustible component of the solid medium inside the object some time after the occurrence of ignition initiated by the lower part of the surface of the object (presented as an ellipse).

![Figure 1](image1.png)

**Figure 1.** The gas velocity field in a porous object during forced filtration after 6 hours after the start of the ignition process.

As it is clear from Figure 1, a larger gas part flows round the hot region and keeps flowing along the edges of the porous object where no combustion has occurred yet.

![Figure 2](image2.png)

**Figure 2.** Degree of conversion of the combustible component of the solid medium field in a porous object during forced filtration after 6 hours after the start of the ignition process.

Increasing the contact area of the solid phase with a gaseous one occurs because of porosity growth. The mass of solid medium in a porous component reduces while the gas rate increases, and due to this the general heat exchange rate increases as well.

Figure 3 shows the dynamics of oxidant mass concentration change in the course of time - oxygen enters into the reaction with fuel in the direction of combustion propagation and, after the region burning out, oxygen enters the region again through an open boundary.
Figure 3. An example of a mass concentration of an oxidizing agent in a porous object during forced filtration after 0.12 (a) and 6 (b) hours after the start of the ignition process.

Figure 4 shows that at the first gas density increases and then starts to decrease. At the initial time stage gas gives a larger part of heat energy to the porous energy which results in density growth.

Figure 4. An example of the gas density function in a porous object during forced filtration 6 hours after the start of the ignition process.

Figure 5. Example of gas temperature in a porous object during forced filtration 6 hours after the start of the ignition process.

Figures 5, 6 present the dynamics of gas temperature and pressure gradients. Temperature is rising in the combustion region and out of the boundaries during the combustion process after which the burned out region becomes cool. The change of oxidant mass concentration (Figure 3) also clearly shows the combustion process propagation. During the combustion of solid porous media, the gas dynamics inside objects is quite complex.
Figure 6. An example of a gas pressure gradient in a porous object during forced filtration 6 hours after the start of the ignition process.

Conclusions
To describe two-dimensional non-stationary flows of viscous thermal conductive gas at filtration combustion of solid porous media, the authors suggest a numerical algorithm. The authors managed to develop a software implementing the suggested numerical method and tested it. The prospective application of the proposed computational model and obtained results is to generate a uniform solver for diffusion reaction systems by means of the finite element method using FreeFem++ [10].

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