On Numerical Model of Two-Dimensional Heterogeneous Combustion in Porous Media

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1 Introduction

Heterogeneous combustion in porous media occurs quite often in nature. From the point of view of mechanics, various objects can be modeled as porous media: soil, peat, rock, debris of destroyed buildings and so on. Smoldering is one of the types of heterogeneous combustion in porous media as heterogeneous chemical reactions take place during smoldering [1]. Many materials can sustain a smoldering reaction, including coal, cotton, duff, peat, wood, and most charring polymers. The most common type of heterogeneous combustion in porous media is peat fire [2]; another example of such combustion is spontaneous combustion of solid waste dumps (landfills). Besides above mentioned examples, the principles of heterogeneous combustion in porous media are used in a various technological processes: burning the municipal and industrial solid waste or another low-calorie fuel, gasification of solid fuels and so on.

When researching the heterogeneous combustion of porous objects in nature we often deal with the process under free convection. Combustion of solid porous medium under free convection was analytically investigated in [3] for counter-flow regime, when the gas and the combustion wave in porous object move in opposite directions, and in [4] for co-flow regime, when the gas moves in the same direction as the combustion wave. In [5] the ability of energy to be concentrated in the front of a co-flow filtration combustion wave in a porous solid was analyzed. In [6] the smoldering of polyurethane foam in natural convection was experimentally studied. Very promising tool for investigating the heterogeneous combustion in porous media is computational modeling. In [7] a one-dimensional transient model of smoldering was presented and solved numerically. A novel computational model of smoldering combustion capable of predicting both countercurrent and cocurrent wave propagation was developed in [8]. A generalized pyrolysis model, Gpyro, for simulating the gasification of a variety of combustible solids encountered in fires was presented in [9]. In [10, 11] Gpyro was expanded to two-dimensional case. Recently in [12] a novel numerical model for investigating the unsteady processes of heterogeneous combustion in porous objects with unknown gas flow rate and gas velocity at the inlet to the object was proposed. The advantage of the proposed model is that it can examine the complex gas dynamics inside the porous object and allows to describe the processes for both forced filtration and free convection, when the flow rate of gas regulates itself. The details of the original numerical method were described in [13]. Using numerical experiment, it was studied in [14] how the gravity field inside the porous object and the pressure difference at the object boundaries, which is caused by the action of gravity on the ambient air, affect the appearance of self-sustaining heterogeneous combustion waves in the object.

In the present work the numerical model, which was previously developed for one-dimensional case in [12-14], is expanded to two-dimensional case and used for solving plane time-dependent problems of heterogeneous combustion in porous objects. In such porous objects the flow rate of oxidant, which enters into the reaction zone in porous object, regulates itself. Used approach enables to solve problems of filtration combustion for both forced filtration and free convection, so it can be efficiently applied for modeling the combustion zones in porous media, which may arise from natural or man-caused disasters.

2 Mathematical model and numerical method

Mathematical model, which is discussed in this paper, can describe the processes of heterogeneous combustion in motionless porous objects, which have some impermeable non-heat-conducting borders and some boundaries opened to the atmosphere. 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 consist 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:

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

where μ is the mass stoichiometric coefficient for oxidizer.

The model is based on the assumption of interacting interpenetrating continua [15] using the classical approaches of the theory of filtration combustion [3-5]. The model includes equations of state, continuity, momentum conservation and energy for each phase (solid and gas); changing the solid phase mass and porosity as well as diffusion of the oxidizer are taken into account. Combustion processes are described by one-step heterogeneous chemical reaction of first order with respect to both arguments. An essential feature of the model is using the equation of momentum conservation for porous media for describing the dynamics of gas; this equation is more correct than the classical Darcy's equation and can be used in a greater range of Reynolds numbers [15]. Another feature of the model is that the dynamic viscosity of gas is temperature dependent by Sutherland’s formula because 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 [16]. In the present work we investigate the two-dimensional (plane) time-dependent gas flow in porous objects with zones of heterogeneous combustion; thus we can write the system of equations for this case, denoting horizontal and vertical coordinates as x_1 and x_2 respectively and summing over repeating indices:

$$\left(\rho_{cf} c_{cf} + \rho_{ci} c_{ci}\right)\frac{\partial T_c}{\partial t} = -\alpha\left(T_c - T_g\right) + Q\rho_{cf0} W + \left(1 - a_g\right)\lambda_c\left(\frac{\partial^2 T_c}{\partial x_1^2} + \frac{\partial^2 T_c}{\partial x_2^2}\right),$$

$$\rho_g c_{gp}\left(\frac{\partial T_g}{\partial t} + v_{gj}\frac{\partial T_g}{\partial x_j}\right) = \alpha\left(T_c - T_g\right),$$

$$\rho_g\left(1 + \chi\left(1 - a_g\right)\right)\left(\frac{\partial v_{g1}}{\partial t} + v_{gj}\frac{\partial v_{g1}}{\partial x_j}\right) = -a_g\frac{\partial p}{\partial x_1} - a_g^2\frac{\mu_1}{k_1}v_{g1} - \rho_{cf0} W v_{g1},$$

$$\rho_g\left(1 + \chi\left(1 - a_g\right)\right)\left(\frac{\partial v_{g2}}{\partial t} + v_{gj}\frac{\partial v_{g2}}{\partial x_j}\right) = -a_g\frac{\partial p}{\partial x_2} - \rho_g \mathrm{g} - a_g^2\frac{\mu_1}{k_1}v_{g2} - \rho_{cf0} W v_{g2},$$

$$\frac{\partial \rho_g}{\partial t}+\frac{\partial \rho_g v_{gj}}{\partial x_j}=\rho_{cf0}W\,, \qquad p=\frac{\rho_g R T_g}{a_g M}\,, \tag{2}$$

$$\rho_g\left(\frac{\partial C}{\partial t}+v_{gi}\frac{\partial C}{\partial x_i}\right)=\frac{\partial}{\partial x_i}\left(\rho_g\, D_g\frac{\partial C}{\partial x_i}\right)-\mu\rho_{cf0}W-\rho_{cf0}WC\,,$$

$$D_g=D_{g0}\left(T_g/273\right)^b\,, \qquad W=(1-\eta)C\,k\,\exp\left(-E/\left(R\,T_c\right)\right),$$

$$\frac{\partial \eta}{\partial t}=W\,, \qquad \rho_{cf}=(1-\eta)\rho_{cf0}\,, \qquad a_g=a_{g0}+a_{cf0}\eta\,, \qquad \mu_1=c_{s1}\frac{T_g^{1.5}}{c_{s2}+T_g}\,.$$

where a is the volume fraction, b is the exponent in the expression for the diffusion coefficient, C is the mass concentration of oxidizer, c is the specific heat, c_{s1} and c_{s2} 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, v_g is the gas velocity, W is the rate of the chemical reaction, α is the constant determining the interphase heat transfer intensity, η is the degree of conversion of the combustible component of the solid medium, λ is the thermal conductivity, μ_1 is the dynamic viscosity of the gas, ρ is the effective density, χ is the coefficient, taking into account the inertial interaction of the phases in their relative motion [15]; 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.

A distinctive feature of the considered model is that the gas 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. So we assume that at the open boundary, where gas flows into the porous object, the gas pressure, gas temperature and mass concentration for the oxidizer are known. At the open boundary, where gas flows out the porous object, the pressure is known. The conditions of heat exchange at the open and impermeable non-heat-conducting borders are also known. Thus the boundary conditions for (2) are as follows:

$$p\big|_{x\in G_1}=p_0(x)\,, \quad \lambda\,\partial T_c/\partial n\big|_{x\in G_1}=\beta\left(T_{g0}-T_c\big|_{x\in G_1}\right),$$

$$T_g\big|_{x\in G_1}=T_{g0} \text{ and } C\big|_{x\in G_1}=C_0\text{, if } \mathbf{v}_{\mathrm{g}}\big|_{x\in G_1}\cdot\mathbf{n}\big|_{x\in G_1}\le 0\,, \tag{3}$$

$$\partial T_g/\partial n\big|_{x\in G_1}=0 \text{ and } \partial C/\partial n\big|_{x\in G_1}=0\text{, if } \mathbf{v}_{\mathrm{g}}\big|_{x\in G_1}\cdot\mathbf{n}\big|_{x\in G_1}>0\,,$$

$$\partial T_c/\partial n\big|_{x\in G_2}=0\,, \quad \partial T_g/\partial n\big|_{x\in G_2}=0\,, \quad \mathbf{v}_{\mathrm{g}}\big|_{x\in G_2}\cdot\mathbf{n}\big|_{x\in G_2}=0\,.$$

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

For the investigation of two-dimensional unsteady gas flow in porous objects with zones of heterogeneous combustion an original numerical method has been developed, which is based on a combination of explicit and implicit finite-difference schemes. This method is the development of earlier proposed numerical algorithm for modeling the one-dimensional problems of heterogeneous combustion in porous objects [12-14]; it is similar to the algorithm for computation of the gas flow through porous objects with heat sources when gas pressure at object boundaries is known [17]. According to the method the energy equations, momentum conservation equation and equation for oxidizer concentration are transformed into the explicit finite difference equations. The gas temperature, solid phase temperature, gas velocity and oxidizer concentration are determined from these equations. The continuity equation is transformed into the implicit finite difference equation. From this equation taking into account the perfect gas equation of state the gas pressure is determined using Thomas algorithm [18]. The effective gas density and the remaining unknown quantities are determined trivially from the perfect gas equation of state and other closure equations. The method is first-order accurate in time and second-order accurate in space. Damping fourth-order terms [18] must be added in the finite difference equations of continuity and momentum conservation. The terms smooth the dispersion errors, but the formal accuracy of the method is unaltered.

The proposed numerical model can be used for solving various problems of filtration combustion for both forced filtration and free convection, for both natural and technological processes.

3 Numerical Results

For illustrating the developed numerical model, consider the following plane time-dependent problem. The porous object with height H and width L is bounded of impermeable non-heat-conducting side walls and is opened at the top (outlet) and at the bottom (inlet). Before the starting moment the pressure at the object inlet and outlet corresponds to the atmospheric pressure at the assigned heights; so there is no air motion in the object. At the starting moment the pressure at the object inlet rapidly increases up to p_{01} and remains constant, and in the place of ignition, which is located at the central part of the object bottom, the temperature of the solid phase reaches a value T_{c0} equal to or exceeding the self-ignition temperature T_{kr}, and burning is started. We use the following parameter values:

$H = L = 10\,\mathrm{m}$, $\rho_{cf0} = 1.1\cdot10^2\,\mathrm{kg/m^3}$, $\rho_{ci} = 6.6\cdot10^2\,\mathrm{kg/m^3}$, $c_{cf} = 1.84\cdot10^3\,\mathrm{J/(kg\,K)}$,

$c_{ci} = 1.84\cdot10^3\,\mathrm{J/(kg\,K)}$, $\alpha = 10^3\,\mathrm{J/(m^3\,K\,s)}$, $c_{gp} = 10^3\,\mathrm{J/(kg\,K)}$, $\lambda_c = 1.2\,\mathrm{J/(m\,K\,s)}$,

$c_{s1} = 1.458\cdot10^{-6}\,\mathrm{kg/(m\,s\,K^{1/2})}$, $c_{s2} = 110.4\,\mathrm{K}$, $k_1 = 10^{-8}\,\mathrm{m^2}$, $\beta = 10\,\mathrm{J/(m^2\,K\,s)}$, $\chi = 0.5$,

$g = 9.8\,\mathrm{m/s^2}$ or $0\,\mathrm{m/s^2}$, $R = 8.31441\,\mathrm{J/(mole\,K)}$, $M = 2.993\cdot10^{-2}\,\mathrm{kg/mole}$, $Q = 8\cdot10^6\,\mathrm{J/kg}$,

$k = 3.16\cdot10^7\,\mathrm{1/s}$ [19], $E = 110\cdot10^3\,\mathrm{J/mole}$ [19], $D_{g0} = 1.82\cdot10^{-5}\,\mathrm{m^2/s}$, $b = 1.724$,

$\mu = 2.667$, $a_{g0} = 0.3$, $a_{cf0} = 0.1$, $T_{g0} = 300\,\mathrm{K}$, $C_0 = 0.23$, $p_{01} = 1.1\cdot10^5\,\mathrm{Pa}$.

In this case, the combustion wave appears and moves upward and to the side walls simultaneously, burning the solid combustible substance completely. Figure 2 shows the example of the solid phase temperature and the field of gas velocity within the porous object.

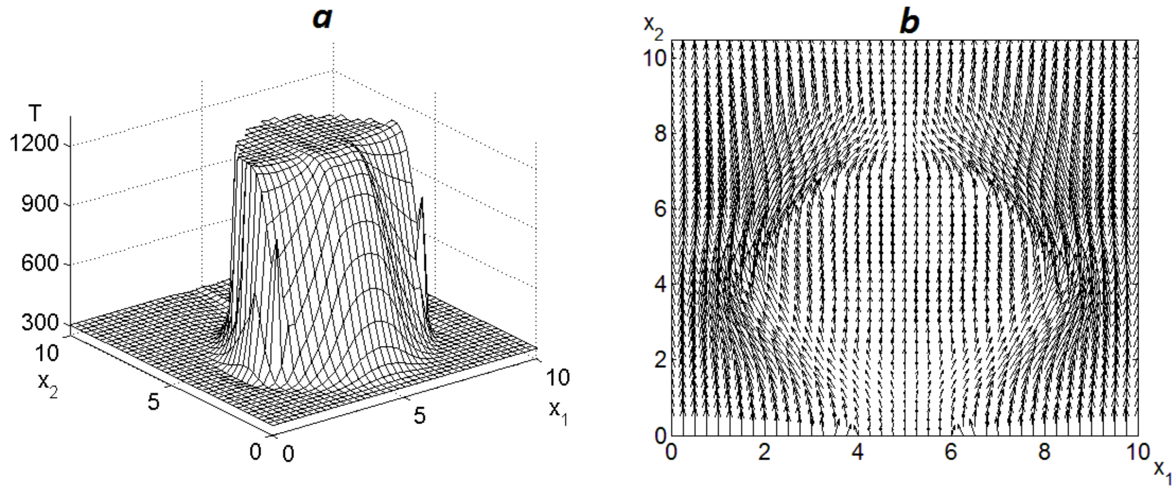

Figure 1. Distributions of the solid phase temperature and the field of gas velocity within the porous object in 5 hours after the time of ignition

As can be seen from the figure, the gas, moving up, tends to go around the heated part of the object and prefers to flow in the cold part of the object, which has not been achieved by the combustion wave. The combustion wave propagation is demonstrated in Fig. 2, which shows the area where the combustible component of the solid medium was completely burnt.

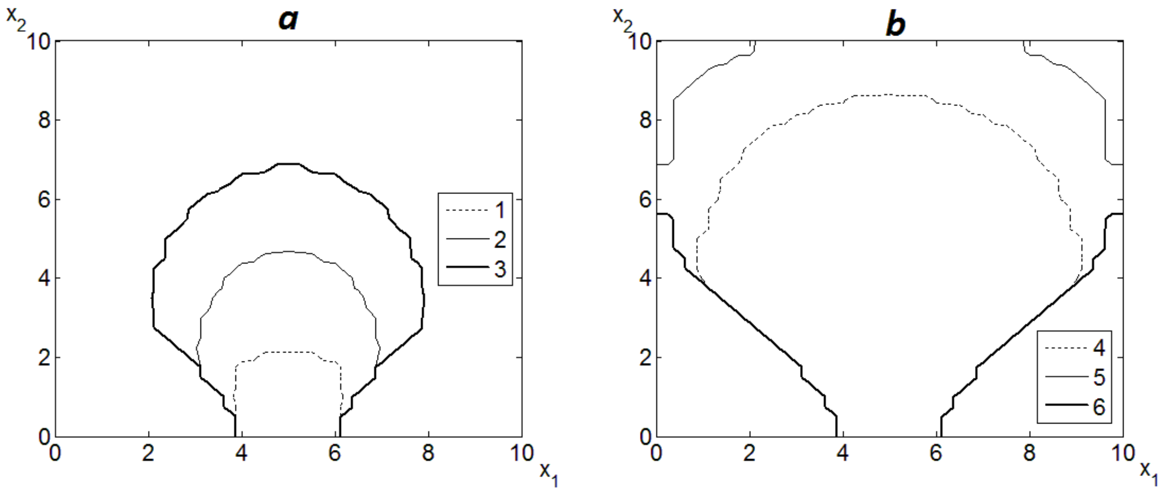

Figure 2. Contours bounding the completely burnt combustible component of the solid medium at different times t after the ignition: t = 1 hour (curve 1), 3 hours (2), 5 hours (3), 7 hours (4), 9 hours (5), and 11 hours (6).

As seen from the figure, the combustion wave moves up and to the side walls of the object. The lower part of the object near the side walls remains unburned, as the combustion wave cannot move across the gas flow or against the flow. The slope of the lines, which separate the burnt part of the object from zones, which cannot be achieved by the combustion wave, depends on the gas pressure at the inlet to the porous object.

When solving the similar problem, but when the place of ignition is located at the center of the object, we can see the same situation: the combustion wave moves upward and to the side walls simultaneously, burning the solid combustible substance completely, and cannot reach the part of the object, located lower the certain lines. At the same time, the slope of these lines depends on the gas flow rate, which is determined by the gas pressure at the inlet to the porous object.

4 Conclusions

The time-dependent problems of heterogeneous combustion in porous objects are considered when the gas pressure at object boundaries is known but the flow rate and velocity of the gas filtration at the inlet to the porous objects are unknown. In such porous objects the flow rate of oxidant, which enters into the reaction zone in porous object, regulates itself. An original numerical method, based on a combination of explicit and implicit finite-difference schemes, has been developed for investigating the unsteady two-dimensional gas flows in such porous objects with zones of heterogeneous reactions. Some plane time-dependent problems of heterogeneous combustion in porous objects have been solved numerically using proposed numerical method. It is shown that gas, moving up, tends to go around the heated part of the object and prefers to flow in the cold part of the object. When the combustion wave propagates inside the porous object, burning the solid combustible substance completely, it cannot reach the part of the object, located lower the certain lines. The slope of these lines depends on the gas flow rate, which is determined by the gas pressure at the inlet to the porous object.

The work was supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003), the Far-Eastern Branch of the Russian Academy of Sciences (project 15-I-4-021), the Far Eastern Federal University. The author would like to acknowledge and thank Academician Vladimir Levin for his encouragement and valuable comments.

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