Smoldering of porous media: numerical model and comparison of calculations with experiment

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Abstract. Numerical modelling of smoldering in porous media under natural convection is considered. Smoldering can be defined as a flameless exothermic surface reaction; it is a type of heterogeneous combustion which can propagate in porous media. Peatbogs, landfills and other natural or man-made porous objects can sustain smoldering under natural (or free) convection, when the flow rate of gas passed through the porous object is unknown a priori. In the present work a numerical model is proposed for investigating smoldering in porous media under natural convection. The model is based on the assumption of interacting interpenetrating continua using classical approaches of the theory of filtration combustion and includes equations of state, continuity, momentum conservation and energy for solid and gas phases. Computational results obtained by means of the numerical model in one-dimensional case are compared with the experimental data of the smoldering combustion in polyurethane foam under free convection in the gravity field, which were described in literature. Calculations shows that when simulating both co-current combustion (when the smoldering wave moves upward) and counter-current combustion (when the smoldering wave moves downward), the numerical model can provide a good quantitative agreement with experiment if the parameters of the model are well defined.

1. Introduction

Combustion of solid porous media is one of the types of filtration combustion; it is quite common in nature and besides is used in some technological processes. From the point of view of mechanics, various objects can be modeled as porous media: for example, peatlands, coal dumps, landfills, grain elevators. When a porous medium burns, the reaction between oxygen and the condensed fuel often occurs directly on the surface of the fuel, that is, the fuel and oxidant are in different phases, so this combustion is heterogeneous. A widespread type of heterogeneous combustion in porous media is smoldering, which can be defined as a flameless exothermic surface reaction propagated with low velocity [1]. Burning of various porous objects during natural or man-made disasters (like peat fire) occurs under free (or natural) convection. In this case the flow rate of gas passed through the porous object is unknown a priori, and only the gas pressure at the object boundaries is known. Smoldering leads to peat megafires, which are the largest and some of the longest burning fires on Earth, cause huge environmental and economic damage, and are responsible for 15% of annual global greenhouse gas emissions [2]. To prevent and eliminate fires in porous objects, it is necessary to study the
dynamics of gas flowing through them, since it can allow to understand how it is possible to limit the flow of oxidant (air) to the combustion zones and, thus, to extinguish the fire.

There are a lot of publications devoted to smoldering and another heterogeneous combustion of solid porous media under free filtration. Analytical investigations of solid porous burning under natural convection were carried out 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. Interesting experimental results of smoldering combustion in some porous materials (cellulose, polyurethane, wood char powder) under free convection were obtained in [5–8]. In [9–14] numerical studies of smoldering combustion under free convection were carried out for various porous materials. At the same time, some important aspects of the smoldering in porous objects under natural conditions remain unstudied. In particular, the detailed gas dynamics in such porous objects has not yet been described due to the complexity of the problem – on the open borders of the simulated object not only the gas flow rate is unknown but also the directions of gas flow.

In the present work a numerical model is proposed for investigating smoldering in porous media under natural convection. The model is the modification of previously developed model [15–16] and can describe more complex conversion of solid porous fuel substance. Computational results obtained by means of the numerical model in one-dimensional case are compared with the experimental data of the smoldering combustion in polyurethane foam under free convection in the gravity field, which were described in [6].

2. Mathematical model and numerical method

Consider a motionless porous object, which has some impermeable non-heat-conducting borders and some boundaries opened to the atmosphere. In the porous medium the self-sustained wave of heterogeneous combustion (smoldering) can propagate. 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 component (or fuel), inert component and solid product of reaction, and at the same time the solid combustible material transforms into gaseous and solid products during the reaction with gaseous oxidizer, so we have the following expression:

\[
\text{Solid fuel} + (\mu_g)\text{Oxidizer} \rightarrow (1+\mu_g-\mu_p)\text{Gaseous product} + (\mu_p)\text{Solid product},
\]

where \(\mu_g\) and \(\mu_p\) are the mass stoichiometric coefficients for oxidizer and solid product respectively.

The model is based on the assumption of interacting interpenetrating continua [17] using classical approaches of the theory of filtration combustion [18] and includes the equations of state, continuity, momentum conservation and energy for each phase (solid and gas):

\[
\begin{align*}
\left(\rho_{cf}c_{cf} + \rho_{ci}c_{ci} + \rho_{cp}c_{cp}\right)\frac{\partial T_c}{\partial t} &= -a(T_c - T_g) + Q\rho_{cf}W + (1-a_g)\lambda_c\Delta T_c, \\
\rho_g\rho_g\left(\frac{\partial T_g}{\partial t} + (v_g \cdot \nabla)T_g\right) &= a(T_c - T_g) + \lambda_g\Delta T_g, \\
\rho_g\left(1 + \chi(1-a_g)\right)\left(\frac{\partial v_g}{\partial t} + (v_g \cdot \nabla)v_g\right) &= -a_g\nabla p + \rho_g a_g^2 \frac{\mu}{k_1}v_g - (1-\mu_p)\rho_{cf}Wv_g, \\
\rho_g\left(\frac{\partial C}{\partial t} + (v_g \cdot \nabla)C\right) &= \nabla \cdot \left(\rho_g D_g \nabla C\right) - \mu_g\rho_{cf}W - (1-\mu_p)\rho_{cf}W_C, \\
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g v_g) &= (1-\mu_p)\rho_{cf}W, \\
p = \frac{\rho_gRT_g}{\alpha_gM}, \\
\frac{\partial \eta}{\partial t} &= W,
\end{align*}
\]
\[ W = (1 - \eta)C \rho g k \exp \left( -\frac{E}{RT_c} \right), \quad \rho_{cf} = (1 - \eta)\rho_{cf0}, \quad \rho_{cp} = \mu_p\rho_{cf0}T, \]

\[ a_g = a_g0 + (a_{cf0} - a_{cpEnd})\eta, \quad D_g = D_g0 \left( \frac{T_g}{273} \right)^b, \quad \mu = c_s1 \frac{T_g^{1.5}}{c_s2 + T_g}. \]

Here \( a \) is the volume concentration, \( b \) is the exponent in the expression for diffusion coefficient, \( C \) is the mass concentration of oxidizer, \( c \) is the specific heat capacity, \( c_{s1} \) 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 release of reaction, \( R \) is the universal gas constant, \( t \) is the time, \( T \) is the temperature, \( g \) is the gas velocity, \( W \) is the rate of chemical reaction, \( \alpha \) is the constant determining the interphase heat transfer intensity, \( \eta \) is the degree of conversion of the combustible component of solid medium, \( \lambda \) is the thermal conductivity (including radiation heat transfer), \( \mu \) is the dynamic viscosity of gas, \( \rho \) is the effective (or bulk) density (i.e., the product of phase density and volumetric concentration), \( \chi \) is the coefficient, taking into account the inertial interaction of the phases in their relative motion [17], \( \nabla \) is the del (nabla) operator, \( \Delta \) is the Laplace operator; subscripts: "0" denotes the initial moment, "c" denotes the condensed phase (solid medium), "End" denotes the end point, "i" denotes the inert component, "f" denotes the combustible component (fuel), "g" denotes the gas, "p" denotes the product.

A distinctive feature of the model is that the equation of momentum conservation for porous media is used, which can be considered as generalization of the classical Darcy’s equation and is convenient for numerical implementation. 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 [19–20]. But the main essential feature of the model is the boundary conditions: 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 object boundaries, which are opened to the atmosphere, we know gas pressure and the conditions of heat exchange. Also at these boundaries we know either gas temperature and the mass concentration for the oxidizer or conditions for gas temperature and oxidizer concentration depending on the directions of the gas flow. At the impermeable boundaries of the object we use the conditions of non-heat-conductivity and impermeability. Thus the boundary conditions for system of equations (2) are as follows:

\[ P_{x \in G_1} = P_{0}(x), \quad \lambda_c \frac{\partial T_c}{\partial n}_{x \in G_1} = \beta \left( T_{g0} - T_{c\mid x \in G_1} \right), \]

\[ T_{g\mid x \in G_1} = T_{g0} \quad \text{and} \quad C_{x \in G_1} = C_0, \quad \text{if} \quad v_{g\mid x \in G_1} \cdot n_{x \in G_1} \leq 0, \]

\[ \frac{\partial T_g}{\partial n}_{x \in G_1} = 0 \quad \text{and} \quad \frac{\partial C}{\partial n}_{x \in G_1} = 0, \quad \text{if} \quad v_{g\mid x \in G_1} \cdot n_{x \in G_1} > 0, \]

\[ \frac{\partial T_c}{\partial n}_{x \in G_2} = 0, \quad \frac{\partial T_g}{\partial n}_{x \in G_2} = 0, \quad v_{g\mid x \in G_2} \cdot n_{x \in G_2} = 0, \]

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

It should be noted, that previously developed mathematical model, which is described in [15–16], is the special case of model (1–3) when \( \mu_p \) is equal to 0. In the present work we investigate the only
one-dimensional processes, as we consider the porous object with height \( H \), which is bounded of impermeable non-heat-conducting side walls and is opened at the top and at the bottom, and at the same time the pressure at the object bottom and top corresponds to the atmospheric pressure at the assigned heights. So, the numerical method for proposed mathematical model (1–3) is very similar to the one used in [15–16] and described in detail in [21]. 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 [22]. The effective gas density and the remaining unknown quantities are determined trivially from the perfect gas equation of state and other closure equations.

3. Comparison of calculations with experiment

Besides of gaining new knowledge, numerous calculations, which were carried out using the mathematical model (1–3) when \( \mu_p \) is equal to 0, showed good qualitative coincidence between obtained computational results and characteristics of filtration combustion described in literature. However, the quantitative coincidence of the computational results with the experimental ones was not previously investigated. There are a lot of parameters in the mathematical model (1–3), some of them have a significant effect on the solution. So, for obtained precise results we should use precise parameter values. But analysis of papers with experimental data showed that the parameters specified in each paper do not allow us to accurately define all the parameter values of the mathematical model (1–3). Therefore, for defining the parameter values of the model, we should use information from different papers. But material used in different experiments on combustion may have different properties. For example, properties of different samples of peat and solid waste can be very different.

However, we assumed that the properties of the polyurethane foam used in various experiments on smoldering can be quite close. And in this way, we can compare the experimental data with the results of our calculations. To define the parameter values of polyurethane foam, we had analyzed a lot of papers and have used data mainly from [6, 9]. Kinetics parameters are obtained from [9] by reducing the two-step mechanism of reactions to the one-step mechanism. The value of the heat release of reaction incorporates the heat loss effect into the heat of combustion. So, we use the following parameters values:

\[
H = 0.15 \text{ m} , \quad \mu_g = 0.536 , \quad \mu_p = 0.1485 , \quad a_{g0} = 0.975 , \quad a_{c\text{End}} = a_{c\text{f0}} = 0.1485 , \\
Q = 2.1 \cdot 10^6 \text{ J/kg} , \quad k = 3.92 \cdot 10^{11} \text{ J/s} , \quad E = 1.4 \cdot 10^5 \text{ J/mole} , \\
\lambda_c = 0.047/0.025 = 1.88 \text{ J/(m K s)} , \quad \lambda_g = 0.034 \text{ J/(m K s)} , \quad \alpha = 10^4 \text{ J/(m}^3 \text{ K s)} , \\
\rho_{c\text{f0}} = a_{c\text{f0}} = 0.16 \cdot 10^3 \text{ kg/m}^3 , \quad \rho_{ci} = 0.025 - a_{c\text{f0}} = 0.10 \cdot 10^3 \text{ kg/m}^3 , \\
c_{c\text{f}} = 1.7 \cdot 10^3 \text{ J/(kg K)} , \quad c_{c\text{i}} = 1.7 \cdot 10^3 \text{ J/(kg K)} , \quad c_{c\text{p}} = 1.7 \cdot 10^3 \text{ J/(kg K)} , \quad c_g = 10^3 \text{ J/(kg K)} , \\
c_{s1} = 1.458 \cdot 10^{-6} \text{ kg/(m s K}^{1/2}) , \quad c_{s2} = 110.4 \text{ K} , \quad R = 8.31441 \text{ J/(mole K)} , \quad g = 9.81 \text{ m/s}^2 , \\
M = 2.993 \cdot 10^{-2} \text{ kg/mole} , \quad D_{g0} = 1.82 \cdot 10^{-5} \text{ m}^2 /\text{s} , \quad b = 1.724 , \quad \chi = 0.5 , \quad \beta = 20 \text{ J/(m}^2 \text{ K s)} , \\
T_{g0} = 300 \text{ K} , \quad C_0 = 0.23 , \quad p_0(0) = 1.00001766 \cdot 10^5 \text{ Pa} , \quad p_0(H) = 10^5 \text{ Pa} .
\]

Some of these parameter values are given in the above mentioned papers; some parameters do not have a strong effect on the solution hypothetically and can be specified approximately (and our calculations confirm this assumption). The main difficulties have arisen in defining the initial volume
concentration of the solid combustible component (fuel) \(a_{cf0}\) and the change in permeability coefficient \(k_1\). Both these parameters have a significant effect on the solution. We suppose, that permeability varies according to the formula \(k_1 = k_{10} + (k_{1End} - k_{10})\eta\), where \(k_{10} = 2.76 \times 10^{-9} \text{ m}^2\) [6], \(k_{1End} = 5.10^{-8} \text{ m}^2\) [6]. Taking into account the variations in heat release of polyurethane foam described in [9], we assume that \(a_{cf0}\) may be from \(0.4 \cdot (1 - a_{g0}) = 0.01\) to \(0.6 \cdot (1 - a_{g0}) = 0.015\).

Computational results obtained by means of the numerical model in 1D case are compared with the experimental data of the smoldering combustion in polyurethane foam under free convection in the gravity field, which were described in [6]. The comparison is carried out in the central part of the porous object, since it was revealed in [6] that smoldering in this zone is free from external effects and is the most representative. Without additional experimental measuring we cannot define very accurate heat losses at the ends of the porous object, so we cannot obtain precise numerical solutions at these zones.

According to the experiment [6], for downward propagation of the smolder wave (counter-current combustion, when the gas and the combustion wave in porous object move in opposite directions) the maximum smolder reaction temperature \(T_{sm}\) in the central zone under natural convection is from 370°C to 380°C, the smolder velocity \(v_{sm}\) is from 3\(\times\)10^{-5} m/s to 4\(\times\)10^{-5} m/s. Figure 1 depicts the maximum smolder reaction temperature and smolder velocity in the central zone of the porous object for different concentration of the solid fuel when the counter-current combustion (downward smoldering) takes place. It should be noted that graphs in this and next figures are obtained when mesh size \(h\) is equal to 0.01. As seen from the figure, the numerical solution depends weakly on the concentration of the solid combustible component and very close to the experimental data.

![Figure 1](image)

**Figure 1.** Maximum smolder reaction temperature \(T_{sm}\) (a) and smolder velocity \(v_{sm}\) (b) versus dimensionless distance from the bottom of the porous object \(x\) when concentration of the solid combustible component \(a_{cf0} = 0.01\) (1), \(a_{cf0} = 0.0125\) (2), \(a_{cf0} = 0.015\) (3) for counter-current combustion (downward propagation of the smolder wave).

According to the experiment [6], for upward propagation of the smolder wave (co-current combustion, when the gas moves in the same direction as the combustion wave) the maximum smolder reaction temperature \(T_{sm}\) in the central zone under natural convection is from 360°C to
390°C, the smolder velocity $v_{sm}$ is from $2.5 \cdot 10^{-5}$ m/s to $3.5 \cdot 10^{-5}$ m/s. Figure 2 shows the maximum smolder reaction temperature and smolder velocity in the central zone of the porous object for different concentration of the solid fuel when the co-current combustion (upward smoldering) takes place. As can be seen from the figure, the numerical solution depends essentially on the concentration of the solid combustible component and rather close to the experimental data. The differences between counter-current and co-current combustion obtained in the calculations may seem strange, however, they agree well with experimental observations. For example, it is said in [8] that upward smoldering is affected by many factors, and operational conditions must be rigidly controlled to achieve repeatability, while downward smoldering is stable. Our numerical calculations demonstrate the same.

![Figure 2](image_url)

**Figure 2.** Maximum smolder reaction temperature $T_{sm}$ (a) and smolder velocity $v_{sm}$ (b) versus dimensionless distance from the bottom of the porous object $x$ when concentration of the solid combustible component $a_{cf0} = 0.01$ (1), $a_{cf0} = 0.0125$ (2), $a_{cf0} = 0.015$ (3) for co-current combustion (upward propagation of the smolder wave).

The calculation accuracy of the used numerical method is demonstrated in figure 3 and figure 4, which show the results of computations with different mesh size. We can conclude that calculations even on rather a coarse grid ($h = 0.025$) give good results. Especially when investigating the smoldering of materials with unstable properties (like peat or solid waste), the use of fine grids may not lead to much more accurate results, since errors in defining the properties of these materials can lead to errors exceeding the accuracy of the calculations.

Thus, the proposed numerical model can provide a good quantitative agreement with experiment if the parameters of the model are well defined. Calculations of the counter-current combustion can be carried out and can give good results without a very accurate definition of some parameters, in contrast to the calculations of the co-current combustion.

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Figure 3. Maximum smolder reaction temperature $T_{sm}$ versus dimensionless distance from the object bottom $x$ when the concentration of the solid fuel $a_{cf0} = 0.0125$ and mesh size $h = 0.025$ (1), $h = 0.01$ (2), $h = 0.0025$ (3) for counter-current combustion.

Figure 4. Temperature of the solid phase $T_c$ versus dimensionless distance from the object bottom $x$ when the concentration of the solid fuel $a_{cf0} = 0.0125$ and mesh size $h = 0.025$ (1), $h = 0.01$ (2), $h = 0.0025$ (3) for co-current combustion.

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