Pore scale numerical simulation of heat transfer in propagating thermal wave during filtration combustion of rich and lean methane-air mixtures

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Abstract. The porous media combustion phenomenon was numerically studied with focus on the heat transfer effect in propagating combustion wave for lean and ultra-rich mixture compositions using the approach when the three-dimensional porous structure and interstitial flow are simulated directly at pore scale with explicit consideration of the thermal interaction between fluid and solid phases including the detailed chemical kinetics model and solid-to-solid radiation. The results demonstrate that irregularity of the porous structure leads to a large spatial variation of the process parameters and the flow inhomogeneity. The most intensive heat sources placed within the cavities where the flow is developed. During the process, the interface heat transfer and radiation contribute to heat recuperation mechanism that leads to thermal non-equilibrium in the combustion wave. The heat is transferred through the bed via radiation layer-by-layer due to restricted visibility of the particles. The numerical data about a local variation of the process parameters were presented. The data of this type can be used for modification of the volume-averaged models within the context of spatial variation consideration. It was shown that there is a correlation between the heat release rate, the interface heat flux, the radiative heat flux, and its root mean square values.

1. Introduction
The porous media combustion (PMC) phenomenon is studied intensively during the last decades because extended flammability limits, low pollutants emission and high stability of combustion that can be achieved during the process [1]. Filling a combustion region with inert porous media leads to energy feedback from the hot products to the incoming mixture via conductivity of the solid matrix and radiation. Such heat recuperation is accompanied by combustion wave formation that stabilizes within porous media or propagates through it. In accordance with the classification proposed by Babkin [2], the wave can propagate through the porous matrix with significantly different velocities. The regime when the wave velocity is the order of $10^{-4}$ m/s was called as the low-velocity regime (LVR). In contrast to the high-velocity regime, the LVR is characterized by strong heat coupling between the flow and solid matrix whereas hydrodynamic interaction is less important. This regime was intensively studied using experimental [3] and numerical [4] techniques.

During the experiments the limited list of measurement methods is available due to non-transparency of the porous media. The most widespread way to analyze the thermal structure near the flame front is based on thermocouples measures. Hence, this type of data does not allow observing local effects such as a difference between fluid and solid temperatures because the registered temperature of covered junction or laid on solid matrix surface junction correlates with only solid temperature. Zheng et al. [3] developed the method to register fluid and solid temperatures separately.
They showed that the difference between $T_i$ and $T_e$ is sufficient. Analysis of the mixture composition in the combustion wave without impact on the process by probe pipes is also unavailable. Alternative non-intrusive methods were used for analysis by Kiefer [5] and Stelzner [6]. Hence, these methods have specific limits and cannot provide the three-dimensional data with high resolution.

Another way to estimate the spatial variation of the heat transfer parameters at the pore scale caused by the structural irregularity of the porous media relates to numerical simulation methods [7]. Most of the numerical investigations are based on a two-temperature volume-averaged model describing the system behavior with the assumption that all parameters are averaged over a macroscopic scale and temporal scale of several hydrodynamic pulsations. This approach provided many important data about the PMC in a wide range of operational parameters [8]. Hence, this approach has a principal limitation that cannot be used for estimation of the local variation of the process parameters such as the velocity or temperature.

To overcome the limitation the approach of representation of the realistic porous media structure at pore scale was developed. Sahraoui and Kaviany [9] showed that the volume-averaged model could not predict local high-temperature spots and flame speed with respect to the flame location. Hackert et al., Jouybari et al., Shi et al. and Sirotkin et al. [10–13] advanced the approach of the pore-scale simulation taking into account solid-to-solid radiation, turbulence effects and randomness of particles packing using two-dimensional models. Authors showed that local variation of process parameters at the pore scale cannot be predicted using the volume-averaged model. Bedoya et al. [14] experimentally and numerically studied lean methane-air flame stabilization in porous media of different geometry. Authors compared the numerical results of volume-averaged and three-dimensional pore-scale simulation approach. It was shown that the volume-averaged approach provides significantly lower thermal flame thickness than in experiments and this approach cannot quantitatively predict temperature profile and burning velocity.

This study is devoted to numerical simulation of the PMC in the low-velocity regime with explicit three-dimensional representation of realistic porous media in the form of a packed bed of spherical particles at the pore scale. The overall objective is to visualize the distribution of the interfacial and radiative heat fluxes at pore scale and estimate heat transfer intensity in the propagating combustion wave depending on the input mixture composition.

2. Methods
The first stage of the study was devoted to the problem of realistic porous structure representation. There are two main approaches when a real sample of the media is scanning using three-dimensional computer tomography technique (sponge-like structures mainly) or generating synthetically using discrete elements method (packed beds mainly). Since in the paper the packed bed of spheres was studied, the second method was used. During the calculation based on the discrete element model to describe particle-to-particle interaction, 5-mm spherical particles were falling into the box under gravity. For verification purposes, the radial porosity profile of the calculated structure was compared with experimental data and empirical equation [15]. The maximum difference was less than 5%.

The next stage related to the computational mesh generation. For packed beds, there is a specific problem with particle-to-particle contact points. Near this region, the mesh cells have a tendency to be distorted due to small angles. Widespread way to overcome the problem is to create an additional geometrical objects near point contacts that have bridge-like shape. Partopour and Dixon [16] developed integrated workflow for pore-scale models based on wrap method when an initial set of surfaces are replacing with a continuous wrapper surface. After the procedure, the conformal fluid-solid volumetric mesh was generated. The total number of cells in the model was about 6 millions.

The mathematical model of the methane-air combustion process within porous media at pore scale should simultaneously describe multicomponent gas flow with chemical reactions, heat transfer between gas and solid porous matrix in which heat transfer by conduction and radiation occurs. In the fluid region, the conservation equations for mass, momentum, energy and species transport equation with unsteady terms were solved. In the solid region, the energy transport equation is solved.
Solid-to-solid radiation significantly contributes to total heat transfer in porous media. Upstream energy transport by radiation influences heat recuperation from high-temperature products to income reactants [17]. Heat exchange between solid surfaces was simulated with the assumptions that all surfaces of the alumina spheres are diffuse and gray without the participation of the gas phase in radiation heat transfer. To simulate radiative heat transfer under the assumptions the model based on view factor calculation was used [18]. Detailed chemical mechanism is a common way to increase the accuracy of major combustion products prediction. The San Diego Mechanism was chosen as a detailed chemical kinetic mechanism of methane-air combustion [19]. The mechanism consists of 57 species and 268 reactions.

Ansys Fluent software was used to solve the governing equations using a finite volume method. The pressure-based solver was used due to low fluid velocity. The coupled algorithm was chosen to solve the momentum and continuity equations together. The second-order upwind interpolation method was chosen for convection terms in all the equations. All diffusion terms were interpolated using a second-order scheme. The second-order accurate implicit temporal discretization scheme was used. Fully implicit time stepping with dual timing formulation was used [20]. This formulation is based on the method when the fluid and solid domains are solving simultaneously with different time steps. Time step in fluid region was set to be $8 \times 10^{-5}$ s, in solid region 0.05 s.

3. Results and discussion

In the study, the porous media combustion of two methane-air mixture composition corresponding to equivalence ratio $\phi = 0.8$ (I case) and 2.5 (II case) was simulated with input velocity of 0.14 m/s (along with y axis). In figure 1, the temperature distribution at the interface (a), the heat release rate ($r$) in the fluid region (b) and the interface (c) and radiative (d) heat fluxes at the interface are shown.

Figure 1. Distribution fields of temperature (a), velocity (b), heat of reaction (c) and CH₄ mole fraction (d) for the case of $\phi = 0.8$. 

It can be seen that the rich mixture composition is characterized by a more sloping temperature profile near the combustion region. This difference relates to the heat release rate of the chemical reaction. The ultra-rich mixture produces less energy due to incomplete combustion with oxygen deficit. The heat release rate for $\phi = 2.5$ is about 43.8% of the $r$ that was predicted for lean mixture composition with $\phi = 0.8$. The combustion wave in the first case is upstream with the propagation velocity of $-0.031 \text{ mm/s}$ whereas in the second case is downstream with the velocity of 0.012 mm/s. Mixture composition has a great influence on the structure of the heat fluxes near the reaction region. Figures 1c and 1d show a distribution of the interface heat flux and the radiative heat flux at the surface of the porous matrix. It can be seen that the parameters are distributed irregularly with strong matching with the porous structure. The region position where the interface heat flux $q_{fs}$ has negative values correlates with the position of the heat release region whereas in lower region heat is transferring from the solid to the mixture. This distribution indicates the mechanism of income mixture preheating in the region before ignition point. Distribution of the radiative heat flux $q_r$ has a more complex structure that explains by used radiation model based on view factor calculation. The model allows considering the visibility of the surfaces of the particles between each other explicitly. Due to that, the radiative heat flux distribution has the wave-shaped form. In the region of the temperature gradient, several nominal layers of the particles are placed. The radiative heat transfer from the most heated region to the preheating region occurs layer by layer with damping. Such structure of the heat fluxes distribution takes place for both cases. But the intensity of the heat transfer is smaller for the case of an ultra-rich mixture.

In figure 2a the fluid and solid temperature profiles are shown for both cases ($T_f$ and $T_s$ profiles are shifted to the right by 20 mm for better visibility). These profiles are the temperature values averaged over cross sections. It can be seen that there is sufficient thermal non-equilibrium between the phases. This difference is a specific feature of the PMC and is the result of heat recuperation mechanism. In figure 2a the preheating region is denoted by I. Here, the heat stored by solid matrix transfers to the fluid. In the region II the reaction is occurring. The heat energy released from the chemical reaction transfers to the solid matrix and then to the preheating region via solid conductivity and radiation. In the region III a thermal relaxation occurs. The same mechanism can be observed for ultra-rich conditions. Hence, the length of the thermal wave in this case is larger. The thermal flame thickness based on averaged fluid temperature $T_f$ is 6.75 mm for lean mixture and 13.5 mm for the ultra-rich mixture. So, the thermal flame thickness correlates with averaged heat release rate: $\delta \propto r$ with the accuracy of 12.5%. The RMS (root mean square) values of $r$ describe it spatial variation at the cross section. The RMS profiles for both cases are shown in figure 2b by dotted curves and denoted as $r_{\text{rms}}$. The RMS values are proportional to their magnitude with coefficient about unity.

**Figure 2.** Temperature profiles (a) and heat release rates (b) for the cases of $\phi = 0.8$ and 2.5.
Figure 3a shows the averaged interface heat flux profiles $q_{fs}$. The profiles have wave-shaped form in the combustion region with the direction changing near the ignition point. Such form is the result of heat recuperation mechanism: before the ignition, the heat flux is directed from the solid matrix to the fluid and vice versa. The magnitude of the interface heat fluxes before and after the flame front is not equal due to heat release region position. The maximum flux is located near the maximum heat release rate. In the preheating region, the heat energy does not release but only transfer from the reaction zone. The maximum RMS value $q_{fs,rms}$ is equal maximum absolute value with 5% accuracy for both cases as it was observed analogously to the heat release rate $r$. The averaged radiative heat flux profiles have a similar but reversed form. Broken shape of the curves is the result of the local porous structure. The RMS values of $q_r$ are larger than their absolute values. For the lean mixture $q_{r, rms} \approx 2q_r$ and $q_{r, rms} \approx 2.8q_r$ for the ultra-rich mixture composition near reaction zone. The radiative heat flux demonstrates the largest spatial variation in comparison with other estimated parameters.

**Figure 3.** Interface (a) and radiative (b) heat fluxes for the cases of $\phi = 0.8$ and 2.5.

4. Conclusion

At the local scale, the parameters distribution has large spatial variation due to an irregularity of the porous structure. The flame front has the shape of combustion cells that form the structure different from planar. The difference in the local wave shape does not lead to dissociation of the front under considered regimes due to compensation of the thermal inhomogeneity by the radiative and convective heat fluxes. Spread of the local heat sources along flow direction as well as the porous structure irregularity leads to the local variation of the interface heat flux that has a strong coupling with a shape of the flame front. The largest spatial variation is observed for the radiative heat flux due to the complex shape of the porous matrix surface. The averaged radiative heat flux profile reflects the local structure of the particles. The interface heat transfers, the conductivity of the porous matrix and the radiation have an important role in heat recuperation mechanism. In the combustion wave, the thermal non-equilibrium between fluid and solid phases is obvious. Averaged thermal flame thickness is proportional to the averaged heat release rate.

Input mixture composition has a great influence on the combustion process. The lean mixture is characterized by total methane consumption and the high heat release rate whereas during ultra-rich mixture combustion major species in the exhaust gas are $H_2$ and CO diluted by nitrogen. Oxygen deficit leads to the significantly lower heat release rate. Such a difference leads to different behavior of the combustion wave. In the case of the lean mixture the wave is upstream whereas in the case of the ultra-rich mixture the wave is downstream. The simplest conception about the balance between heat fluxes in the combustion wave can explain this dependence. Input fluid flow takes the heat energy in the preheating region via convective heat transfer with intensity $q_1$. Conductive heat flux in the porous
matrix and radiation deliver the energy from the high-temperature region in the preheating region with intensity \( q_1 \). If \( q_1 > q_2 \) the wave is downstream, \( q_1 < q_2 \) the wave is upstream [8]. If the fluxes are equal the wave stabilizes within porous media.

The pore-scale approach provides numerical data about the local variation of the process parameters. The data of this type can be used for modification of the volume averaged models within the context of spatial variation consideration. It was shown that there is a correlation between the heat release rate, the interface heat flux, the radiative heat flux and their RMS values. As it was proposed by Bedoya et al. [14] spatial fluctuations of the process parameters can be taken into account within the framework of the volume-averaged approach using a presumed shape probability density function which can be constructed based on the pore-scale simulation data.

Acknowledgment

The reported study was funded by Russian Foundation for Basic Research according to the research project № 18-31-00071.

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