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Transient Numerical Simulation of Combustion in Inert Porous Media

This paper presents methods for the time-dependent numerical solution of a two-dimensional model governing combustion in inert porous media. The spatial discretization is based on a mixed finite element method for the flow problem and a cell-centered finite volume scheme for the transport equations. Some results of numerical simulations show the influence of a jump in the porosity of the solid matrix on the localization of the combustion zone.

1. Introduction

Combustion in inert porous media is gaining increasing interest, as there are several advantages in comparison with combustion in free flames. The position of the flame and the temperature distribution can be controlled better by cooling of the porous matrix, which leads to lower emission rates. Furthermore, porous burners are able to generate heat with a larger modulation range and can be constructed in a more compact way [5].

A porous combustion device consists of a metal cylinder filled with ceramic grains or a ceramic foam. The outer wall of the cylinder can be cooled by forced convection with water. The porous medium has low porosity near the inlet (region A), and high porosity in the remaining part (regions B and C). A mixture of methane and air enters at the inlet and combusts in the part with high porosity.

Numerical simulations can contribute to the development and optimization of porous burners. Such computations are based on an appropriate mathematical model. After introducing this model we want to present numerical methods for the discretization of the governing equations and the solution of the resulting system of nonlinear equations. Finally, we present some results of numerical simulations that show how the jump in the porosity and the cooling of the outer wall contribute to the localization and stabilization of the flame.

2. The mathematical model

We restrict our considerations here to the case of an exothermic one-step reaction mechanism. Then the mathematical model consists of the following equations, which can be derived by the method of volume averaging [4].

The flow in the porous medium is governed by the equations

$$
\phi \partial_t \rho + \text{div} (\mathbf{m}) = 0
$$

(1)

$$
\frac{1}{\rho} \left( \frac{\mu}{k} + \frac{c_F}{\sqrt{k}} |\mathbf{m}| \right) \mathbf{m} + \nabla p = 0
$$

(2)

$$
p = R_0 T_g \frac{p}{W}
$$

(3)

The unknowns in this system are the density \( \rho \), the pressure \( p \) and the mass flux density \( \mathbf{m} \). The porosity \( \phi \) and permeability \( k \) of the porous medium, the viscosity \( \mu \) of the gas mixture and the molecular weight \( W \) of the species are known as well as the Forchheimer constant \( c_F \) and the universal gas constant \( R_0 \). The Darcy–Forchheimer equation (2) is a nonlinear extension of Darcy’s law for flow with higher velocity, could be used together with the equation of state (3) to express \( \mathbf{m} \) in terms of \( \rho \), leading to one parabolic equation for the flow problem.

The following equations

$$
\phi \partial_t (\rho y) + \text{div} (\mathbf{m} y - \phi D \nabla y) = -\phi \dot{\gamma}
$$

(4)

$$
\phi c_p \partial_t (\rho T_g) - \phi \partial_t p + c_p \text{div} (\mathbf{m} T_g) - \text{div} (\phi \lambda_y \nabla T_g) = \phi Q \dot{\gamma} - ha(1-\phi)(T_g - T_s)
$$

(5)

$$
(1-\phi) \rho_c c_s \partial_t T_s - \text{div} ((1-\phi) \lambda_s \nabla T_s) = ha(1-\phi)(T_g - T_s)
$$

(6)

describe the transport of the reactant (4), and heat in the gas mixture (5) and the solid (6), resp.. The unknowns
here are the mass fraction of the reactant $y$, the temperature of the gas mixture $T_g$ and the temperature of the solid $T_s$. The specific heat $c_p$ and heat conductivity $\lambda_g$ of the gas mixture, the specific heat $c_s$, heat conductivity $\lambda_s$ and density $\rho_s$ of the solid, the mass diffusion coefficient $D$ and the heat of reaction $Q$ are known. The reaction rate is given by the Arrhenius model

$$\dot{r} = B \rho y e^{-E/R_0 T_s},$$

where $B$ is the frequency factor and $E$ the activation energy.

The heat exchange between the gas mixture and the porous medium is supposed to be proportional to the temperature difference with a heat transfer coefficient $h$. Because of the high specific surface $a$ of the porous medium, this heat exchange term is much larger than the other terms in equations (5) and (6). Thus we may assume that the temperature of the gas mixture and the solid are equal ($T_g = T_s =: T$), leading to the effective heat equation

$$\partial_t ((\phi c_p \rho + (1 - \phi) c_s \rho_s) T) - \phi \partial_i p + \text{div} (c_p m T - (\phi \lambda_g + (1 - \phi) \lambda_s) \nabla T) - \phi Q \dot{r} = 0,$$

where $c_p$, $c_s$ and $\rho_s$ are assumed to be constant.

3. Discretization and solution of the two-dimensional time-dependent problem

Using the method of lines we first have to discretize the governing equations in space. To this end we introduce a decomposition $T_h$ of the computational domain $\Omega$ into triangular elements $K$. For every $K \in T_h$ we denote by $P_k(K)$, $k \geq 0$, the set of polynomials of degree $\leq k$ on $K$. For every edge $e \in \partial K$, being the set of edges of $T_h$, we define a unique unit normal vector $n_e$.

To get a good approximation for the mass flux density $m$, which appears also in equations (4) and (7), we use the mixed finite element method on Raviart–Thomas elements of lowest order (see e.g. [2]) for the spatial discretization of equations (1) and (2), as proposed in [3]. Thus $m$ is approximated by $m_h \in V_h$, where

$$V_h := RT_0(\Omega; T_h) := \left\{ v_h \in H(\text{div}; \Omega) \mid v_h|_K \in RT_0(K) \quad \forall K \in T_h \right\}$$

and $RT_0(K)$ is defined by

$$RT_0(K) := \left( P_0(K) \right)^2 + \frac{x^2 + y^2}{2} P_0(K).$$

Note that any $v_h|_K \in RT_0(K)$ is uniquely defined by the normal components of the mass flux across the edges of $K$

$$v_e := \int_{\partial K} v_h|_K \cdot n_e \, ds, \quad e \subset \partial K,$$

and that the property $v_h \in H(\text{div}; \Omega)$ requires the continuity of these mass flux values. This continuity is achieved by using a basis $\{ w_e \}_{e \in E_h}$ of $V_h$ satisfying

$$\int_{\partial K} w_e \cdot n_f \, ds = \begin{cases} 1 & \text{if } e = f \\ 0 & \text{if } e \neq f \end{cases}.$$ 

The degrees of freedom are therefore given by the mass flux values $v_e$, $e \in E_h$. Corresponding to the choice of $V_h$ the pressure $p$ is approximated by $p_h \in Q_h$, where $Q_h$ is defined by

$$Q_h := \{ q_h \in L^2(\Omega) \mid q_h|_K \in P_0(K) \quad \forall K \in T_h \}.$$

Using the mixed finite element method we get the same approximation order for the mass flow rate $m$ and the pressure $p$. Furthermore it ensures local mass conservation on each element, a property which is well desired for this kind of equations.

The mass fraction of methane $y$ and the temperature $T$ are also approximated by elements of $Q_h$. To save computational cost, we do not compute the corresponding fluxes directly, but discretize equations (4) and (7) by a cell centered finite volume scheme which is strongly related to the mixed finite element method [1]. Hence this ensures local mass conservation, too. The flux across the edges of the elements is computed using an upwind scheme for the convective part and central differences for the diffusive part. Unfortunately this inhibits the use of triangles with obtuse angles [1], a fact which has to be taken into account for the construction of the decomposition $T_h$.

Having performed the discretization in space we end up with a system of ordinary differential equations for the degrees of freedom. This system is integrated in time by an implicit Euler or Crank–Nicolson method. The time
step size can vary in a certain range. This variation is controlled by the convergence behaviour of the nonlinear solution process.

The resulting nonlinear system of equations is solved in the following way:

We do not consider the fully coupled system, but decouple the flow problem from the transport equations. The resulting two subsystems are solved in an alternating iteration, which terminates, when both solution processes are converged. Each subsystem is linearized by a generalized Newton method and the resulting linear problems are solved by appropriate multigrid methods.

4. Influence of jump in porosity

Below we present some results of numerical simulations that show how the jump in the porosity of the solid matrix contributes to the stabilization of the flame.

To this end we do some computations on a simple rectangular domain representing the upper half of a porous burner. The lower boundary (ΓS) is assumed to be a line of symmetry, while the upper boundary (ΓC) corresponds to the cooled outer wall. The cooling at the boundary part ΓC1 is stronger than at ΓC2, represented by a larger heat transfer coefficient.

Nearly all coefficients remain unchanged for these computations. Only the values for porosity and permeability are varied. The progression of the simulations is as follows: Beginning with a stationary flow field, the combustion process is started by an artificial heat source in the ignition zone. After the ignition of the fuel (reactant), this artificial heat source is switched off and the simulation is continued until a stationary solution is reached. Depending on the choice of the porosity values, the resulting solutions differ significantly.

For a configuration with jump in the values for porosity and permeability (φ = 0.3, k = 10⁻⁸ m² in region A and φ = 0.8, k = 10⁻⁷ m² in region B) the combustion zone is localized near the boundary between region A and B. It cannot move towards the inlet, because the heat loss in region A is too strong due to the high heat conductivity. The steady state solutions for T and y are shown in the following figures.

Temperature distribution for jump in porosity  Mass fraction of fuel for jump in porosity

The use of constant values for porosity and permeability leads to totally different results. For a value of φ = 0.3 and k = 10⁻⁸ m² both in region A and in region B, the combustion process dies out after switching off the artificial heat source. In this case the effective heat conductivity is high in both regions, leading to a stronger heat loss. Hence more heat is lost through cooling of the wall than produced by the combustion process.
Let us finally consider constant values of \( \phi = 0.8 \) and \( k = 10^{-4} \text{m}^2 \). In this case the effective heat conductivity is low in region A, too. Thus the produced heat cannot be led away fast enough, the combustion zone moves towards the inlet and finally reaches the inlet. The corresponding steady state solution shows this behaviour.

![Temperature distribution for constant porosity of 0.8](image1.png) ![Mass fraction of fuel for constant porosity of 0.8](image2.png)

Further simulations performed using other constant values for the porosity and permeability show either the same behaviour as those for \( \phi = 0.3 \) or the same behaviour as those for \( \phi = 0.8 \). In fact no constant values of porosity and permeability can be found for which the fuel gets completely combusted. Hence a jump in the porosity contributes significantly to the localization of the combustion zone inside the porous burner.

5. Conclusion

We presented a model for combustion in inert porous media. We proposed numerical methods for the discretization of these equations and for the solution of the resulting nonlinear system of equations. With the aid of this algorithm we performed several simulations for porous media with and without jump discontinuity in the porosity. The results of these simulations show that a jump in the porosity of the solid matrix contributes significantly to the localization of the flame.

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6. References


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