Numerical Bifurcation Analysis of Premixed Combustion in Porous Inert Media

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Abstract. In this paper we perform a numerical bifurcation analysis of a one-dimensional problem arising in premixed combustion in porous inert media. The analysis shows that multiple steady solutions may occur, that a minimal mass flow rate is required for steady combustion, and that solutions with complete combustion exist for a large range of mass flow rates. Moreover, we show that a jump discontinuity in porosity and cooling contributes to the stability of the combustion zone. The one-dimensional results are compared with computations for a corresponding two-dimensional problem. The qualitative agreement between the solutions is good along the cooling boundary, and satisfactory along the axis of symmetry. The one-dimensional problem can therefore be used as preparation for a more complex two-dimensional simulation.

1 Introduction

Premixed combustion in porous inert media can be utilized for heat generation at a domestic scale, like in a central heating system. This technique has some advantages over heat generation with conventional open-flame burners. The main advantages are the large modulation range of generated power and the low emission rates of nitrogen oxides (NOx). The porous medium can be a ceramic foam or consist of ceramic particles. It serves to extract heat from the reaction zone, thereby lowering the temperature and reducing NOx formation. Cooling of the porous matrix is also used to stabilize the position of the combustion zone over a large power range. With premixed combustion in porous inert media, relatively high power densities can be achieved, which makes compact constructions of porous burners possible.

Several authors have performed numerical studies for one-dimensional models of porous inert media burners, e.g. [8,4,5]. In these models the porous medium is homogeneous, and radiation is the main stabilizing mechanism controlling the flame. In [8] and [5] steady-state solutions are computed using a fixed flame temperature at a particular point in the computational domain. The resulting problem is then solved for the corresponding burning speed, which is viewed as an eigenvalue. In [4] transient simulations are performed to obtain steady solutions for a prescribed mass flow rate. In these computations no flame temperature at a fixed point needs to be specified.
A porous burner with a different construction has been investigated experimentally by Trimi and Durst [9]. This type of burner is characterized by two regions having different porosity and thermal properties, which are connected by a jump discontinuity. The region at the upstream end has a lower porosity than the one at the downstream end, which serves as a combustion chamber. An important difference with the burner type considered in [8,4,5] is that the outside wall of the burner is cooled convectively by water. The heat conduction towards the wall plays here a crucial role in the stabilization of the flame.

In the present paper we investigate a model corresponding to the latter type of burner. For this model we study the effect of the jump discontinuity in porosity and cooling on the stability of the flame. The combustion is modelled by a single-step, irreversible reaction. The effect of radiation from the porous solid is disregarded.

For the computation of a steady one-dimensional solution we follow an approach that differs from that in [8,4,5]. Since we expect that there are multiple steady solutions, we use a parameter continuation method known from bifurcation theory. Because with this method we do not need to specify a fixed flame temperature, it is very suitable for studying the stabilizing effect of the inhomogeneity in the porous medium on the combustion zone. Moreover it yields the dependence of the multiplicity of solutions on a selected continuation parameter, like e.g. a Danköhler or Peclet number. For example, we will show that there is a minimum Peclet number (proportional to mass flow rate) below which no steady-state solution with combustion exists.

The one-dimensional results are compared with a steady-state solution of a corresponding two-dimensional problem. The two-dimensional solution is obtained by transient simulation of the model including the flow equations.

The outline of this paper is as follows. In Sect. 2 we present the mathematical model for premixed combustion in porous inert media. From this multidimensional model we derive a simplified one-dimensional model, which we will use for our bifurcation analysis. To motivate that multiple solutions may occur, we give an asymptotic analysis for high activation energy in Sect. 3. Next we present in the same section the results of the numerical bifurcation analysis. In Sect. 4 we compare the one-dimensional results with a corresponding two-dimensional problem. We summarize our conclusions in Sect. 5.

2 Basic Equations governing Premixed Combustion in Porous Inert Media

In this section we present the model for premixed combustion in porous inert media and derive a one-dimensional simplified model.
2.1 General model

In Fig. 1 we have schematically depicted the geometry of the upper half of a porous inert media burner. The gas mixture enters at the inflow boundary $\Gamma_i$ at the left, and the combustion products leave the burner at the outflow boundary $\Gamma_o$ at the right. The upper lateral boundary is an impermeable wall and is cooled, the lower lateral boundary is an axis of symmetry. The porosity in region A is smaller than in B, and the cooling at boundary $\Gamma_{C1}$ is higher than the cooling at $\Gamma_{C1}$.

![Geometry of a porous inert media burner.](image)

Recently we have developed a multi-dimensional model for combustion in porous inert media, including equations governing the flow in a porous medium [7]. The flow in the porous medium is governed by the continuity equation

$$\phi \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = 0, \quad (1)$$

the Darcy–Forchheimer equation,

$$- \nabla \mathbf{p} = \frac{\mu}{k} \mathbf{v} + \frac{c_F}{\sqrt{k}} \rho |\mathbf{v}| \mathbf{v}, \quad (2)$$

and the equation of state

$$p = R T \frac{\mu}{W}, \quad (3)$$

where $\rho$ is the mass density of the gas mixture, $\mathbf{v}$ the Darcy velocity, $p$ the pressure, and $T$ the temperature of the gas mixture. Here $\mu$ and $W$ are the viscosity and the average molecular weight of the gas mixture, $c_F$ the Forchheimer coefficient, and $R$ the universal gas constant. The porosity and permeability of the porous medium are denoted by $\phi$ and $k$, respectively.

We consider a single-step reaction mechanism, so that we only have one species transport equation for the mass fraction $y$ of the reactant.

$$\phi \rho D_t y = \text{div}(\phi \mathbf{D} \nabla y) - \phi \dot{r}, \quad (4)$$

where $D_t = \partial_t + (v/\phi) \cdot \nabla$ denotes the material derivative and $D$ is the mass diffusion coefficient. The mass consumption rate $\dot{r}$ of reactant is given by

$$\dot{r} = B \rho y e^{-E/RT}, \quad (5)$$
where $E$ is the activation energy and $\mathcal{B}$ the frequency factor.

In the case that the solid and gas phases are not in local thermodynamic equilibrium, we have to consider two separate equations for heat transport:

$$ \phi \rho c_p \frac{D_t T_g}{c_s} - \phi \frac{\partial_t}{\partial_t} = \text{div} \left( \phi \lambda_g \nabla T_g \right) + \phi Q \tilde{r} - \rho a(1 - \phi)(T_g - T_s) , \tag{6} $$

and

$$ (1 - \phi) \rho_s c_s \frac{\partial_t T_s}{c_s} = \text{div} \left( (1 - \phi) \lambda_s \nabla T_s \right) + h a(1 - \phi)(T_g - T_s) , \tag{7} $$

where $T_s$ is the temperature in the solid. Here $Q$ is the heat of reaction, $\lambda_g$ and $c_s$ the thermal conductivity and specific heat at constant pressure of the gas mixture, $\rho_s$, $\lambda_s$, and $c_s$ the mass density, thermal conductivity, and specific heat of the solid. The coefficient $a$ in the last term of (6) and (7) is the surface area per volume of solid, and $h$ is the heat transfer coefficient. Because $ha$ is usually very large, we assume $T = T_g \approx T_s$, yielding after addition of (6) and (7)

$$ \phi \rho c_p \frac{D_t T}{c_s} + (1 - \phi) \rho_s c_s \frac{\partial_t T}{c_s} - \phi \frac{\partial_t}{\partial_t} = \text{div} \left( \lambda_{\text{eff}} \nabla T \right) + \phi Q \tilde{r} , \tag{8} $$

where $\lambda_{\text{eff}}$ is the effective thermal conductivity,

$$ \lambda_{\text{eff}} = \phi \lambda_g + (1 - \phi) \lambda_s . \tag{9} $$

The boundary condition for the heat flux at the cooling boundary is modelled by Newton’s law of cooling,

$$ - n \cdot \lambda_{\text{eff}} \nabla T = h_w(T - T_{\text{amb}}) \quad \text{at } \Gamma_{C0} \cup \Gamma_{C1} , \tag{10} $$

where $h_w$ is the heat transfer coefficient of the wall, $T_{\text{amb}}$ the ambient temperature, and $n$ the outward directed normal.

### 2.2 One-Dimensional Simplified Model

From the previously discussed model we derive a simplified one-dimensional steady-state model that we will use in our numerical bifurcation analysis. For a steady and one-dimensional flow, we obtain from (1)

$$ \frac{d}{dx} (\rho v) = 0 , \tag{11} $$

so that the mass flow rate is constant, $\rho v = m_0$. Furthermore, using (2) and (3), it can be shown that the pressure variation is relatively small for practical values of the mass flow rate and temperature. To simplify the one-dimensional model we therefore assume that the pressure is constant, $p = p_0$. The equation of state (3) is then used to eliminate $\rho$ from (5). To model the effect of cooling (see (10)), we introduce a sink term in the heat equation,
which is proportional to $h_w(T - T_{amb})$. Using these simplifications we obtain from (4) and (8)

$$m_0 \frac{dy}{dx} = \frac{d}{dx} \left( \phi D \frac{dy}{dx} \right) - \phi \dot{r}(y, T),$$  

(12)

$$m_0 c_p \frac{dT}{dx} = \frac{d}{dx} \left( \lambda_{eff} \frac{dT}{dx} \right) + \phi Q \dot{r}(y, T) - h_w a_w (T - T_{amb}),$$  

(13)

where $a_w$ is the ratio of the area of the cooling boundary and the volume of the whole domain.

To non-dimensionalize the equations we scale $x$, $T$, and $y$ according to

$$x := \frac{x}{L}, \quad T := \frac{T}{T_0}, \quad y := \frac{y}{y_0},$$  

(14)

where $L$ is the length of the domain, and $T_0$ and $y_0$ are some reference values to be specified later. When the heat transfer coefficient is not zero, we take $T_0 = T_{amb}$. We also define a reference value $\rho_0$ for the density using (3) with $T_k = T_0$ and $p = p_0$. The Peclet and Damköhler number are defined by

$$Pe = \frac{m_0 c_p L}{\lambda_k}, \quad \Delta = \frac{\rho_0 c_p L^2}{\lambda_k} B \exp(-E/RT_0).$$  

(15)

These numbers will be selected later as continuation parameters. We remark that $\Delta$ is the ratio of a characteristic conduction and a characteristic reaction time scale. The other dimensionless numbers, i.e. the dimensionless activation energy, the heat release energy, the characteristic conduction and a characteristic reaction time scale.

Using these definitions, we obtain the following dimensionless equations:

$$Pe \dot{y} - \Delta \dot{r}(y, T),$$  

(17)

$$Pe \dot{T} - \left( \tilde{\lambda}_{eff} \dot{T} \right) = \phi \beta \Delta \dot{r}(y, T) - \tilde{h}_{eff}(T - 1),$$  

(18)

where primes denote differentiation with respect to $x$,

$$\dot{r} = \frac{y}{T} \exp(\theta - \theta/T),$$  

(19)

and

$$\tilde{\lambda}_{eff} = \frac{\lambda_{eff}}{\lambda_k} \quad \text{and} \quad \tilde{h}_{eff} = \frac{h_w a_w L^2}{\lambda_k}.$$  

(20)

This coupled system of equations for $y$ and $T$ is analysed in the next section.
3 Analysis of Steady-State One-Dimensional Problem

To illustrate that system (17)–(18) may have multiple solutions we use an asymptotic analysis for high activation energy.

3.1 Activation Energy Asymptotics

We consider equations (17)–(18) for $0 < x < 1$ together with the boundary conditions

$$T(0) = 1, \quad y(0) = 1, \quad T'(1) = 0, \quad y'(1) = 0.$$  \hspace{1cm} (21)

This problem is analysed for the case without cooling, i.e. $\overline{h}_{\text{eff}} = 0$, and constant porosity $\phi$. We assume that the activation energy is large, so that $\epsilon = 1/\theta$ is a small parameter. We seek solutions in the form of the expansions

$$T = 1 + \epsilon S, \quad y = 1 - \epsilon Y, \quad \epsilon \ll 1.$$  \hspace{1cm} (22)

Furthermore, we assume that the mass flow rate and $\Delta$ are small, such that

$$\text{Pe} = O(\epsilon) \quad \text{and} \quad \Delta = O(\epsilon) \quad \text{as} \quad \epsilon \to 0.$$  \hspace{1cm} (23)

Then substituting these expressions into (17)–(18) and collecting lowest-order terms, we observe that the heat equation decouples from the species equation. For the temperature deviation $S$ we obtain

$$\begin{cases} -S'' = \delta \exp(S), & 0 < x < 1, \\ S(0) = 0, & S'(1) = 0, \end{cases}$$  \hspace{1cm} (24)

where

$$\delta = \frac{\Delta}{\epsilon} \frac{\beta \phi}{\lambda_{\text{eff}}}.$$  \hspace{1cm} (25)

The problem given by (24) is known as the Gelfand problem. For an analysis of this problem in more dimensions we refer to Bebernies and Eberly [2]. Provided a solution exists, problem (24) can be solved by multiplication of the equation for $S$ by $S'$ and subsequent integration. It yields an expression $S = S(x; \gamma, \delta)$, where $\gamma = S(1)$, and a relation between $\gamma$ and $\delta$,

$$\delta = 2e^{-\gamma} \text{arctanh}^2 \sqrt{1 - e^{-\gamma}}.$$  \hspace{1cm} (26)

For sufficiently small $\delta > 0$ there are two values of $\gamma = S(1)$ that satisfy (26) in that case two solutions exist corresponding to one and the same $\delta$. 

3.2 Numerical Bifurcation Analysis

Because the steady-state problem may not have a unique solution depending on the parameter values, we use a parameter continuation method for the computation of steady-state solutions.

We consider system (17)–(18) for \(0 < x < 1\) together with the boundary conditions (21), except that the condition for \(\dot{T}(0)\) is replaced by the equilibrium condition

\[
\text{Pe}\, \dot{T}(0) - \tilde{\lambda}_{\text{eff}} T'(0) = \text{Pe}.
\]  

(27)

This condition expresses that the total inflowing heat flux is constant, corresponding to a convective heat flux with constant temperature \(T = 1\). The porosity \(\phi\) and the heat transfer coefficient \(h_w\) are assumed to have a jump discontinuity at \(x = x_i \in (0, 1)\),

\[
\phi = \begin{cases} 
\phi_0 & \text{if } x < x_i, \\
\phi_1 & \text{if } x > x_i,
\end{cases}
\quad \text{and} \quad
h_w = \begin{cases} 
h_{w;0} & \text{if } x < x_i, \\
h_{w;1} & \text{if } x > x_i.
\end{cases}
\]  

(28)

We remark that as a consequence \(\tilde{\lambda}_{\text{eff}}\) and \(\tilde{h}_{\text{eff}}\) are discontinuous at \(x = x_i\).

For the computation of the bifurcation diagrams and the corresponding steady solutions, we make use of the programme AUTO [3]. The boundary value problem under consideration is discretized by an orthogonal collocation method using piecewise polynomials. The programme automatically adapts the mesh to equitably distribute the local discretization error. Pseudo-arclength continuation is used for continuation of a selected parameter. The resulting system of nonlinear equations is solved by a Newton-Chord iteration.

Motivated by the asymptotic analysis in Sect. 3.1, we select the Damköhler number \(\Delta\) as continuation parameter and keep the other parameters fixed \(\text{Pe} = 1000\). The parameter values used in the computation are given in Tab. 1. The data for the gas mixture correspond to methane-air combustion at an equivalence ratio of 0.91

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<tr>
<td>(a_w)</td>
<td>12.5 m(^{-1})</td>
<td>(E)</td>
<td>1.256 (\cdot) 10(^7) J/mol</td>
<td>(y_0)</td>
<td>0.05</td>
</tr>
<tr>
<td>(B)</td>
<td>1.8 (\cdot) 10(^{-8}) s(^{-1})</td>
<td>(L)</td>
<td>0.32 m</td>
<td>(\phi_0)</td>
<td>0.3</td>
</tr>
<tr>
<td>(c_p)</td>
<td>1005 J/kg K</td>
<td>(Q)</td>
<td>5.0 (\cdot) 10(^7) J/kg</td>
<td>(\phi_1)</td>
<td>0.8</td>
</tr>
<tr>
<td>(D)</td>
<td>5.0 (\cdot) 10(^{-3}) kg m/s</td>
<td>(R)</td>
<td>8.314 J/mol K</td>
<td>(\lambda_e)</td>
<td>0.024 W/Km</td>
</tr>
<tr>
<td>(h_{w;0})</td>
<td>2000 W/Km(^2)</td>
<td>(T_0)</td>
<td>298 K</td>
<td>(\lambda_m)</td>
<td>36 W/Km</td>
</tr>
<tr>
<td>(h_{w;1})</td>
<td>50 W/Km(^2)</td>
<td>(x_1)</td>
<td>0.25</td>
<td>(\rho_0)</td>
<td>1.18 kg/m(^3)</td>
</tr>
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The computation is started at $\Delta = 0$ with the trivial solution $T \equiv 1$, $y \equiv 1$. The resulting bifurcation diagram is shown in Fig. 2. We use the maximum temperature as measure in the diagram.

The solution branch in Fig. 2 is continued from the starting point at label 1 to the right. At a value of $\Delta \approx 6.0$ there is a turning point (outside the diagram) at which the branch continues to the left along the middle branch. At the point indicated with label 4, the branch turns to the right and continues along the upper branch. The solutions labeled with 1, 3, and 5, are lying each on a different solution branch. All three correspond to $\Delta = 8.8 \cdot 10^{-11}$, which is the Damköhler number that is found when the physical parameters of Tab. 1 are substituted into the definition of $\Delta$ in (15). The corresponding temperature and mass fraction profiles are shown in Fig. 3.

![Fig. 2. Bifurcation diagram: maximum temperature versus Damköhler number (Pe = 1000)](image)

From the mass fraction profiles in Fig. 3(b) we observe that the lower branch in Fig. 2 represents steady solutions with negligible combustion, the middle branch solutions with partial combustion, and the upper branch solutions with full combustion. The solutions with partial combustion are supposedly unstable under time-dependent perturbations.

Next, we study the influence of variations in the Peclet number, which is proportional to the mass flow rate. We select Pe as the continuation parameter and keep other parameters fixed. Taking solution 3 at the middle branch in Fig. 2 as starting point, the Peclet number is continued in both directions up to $\text{Pe} = 3000$, yielding the upper two branches in the bifurcation diagram in Fig. 4. The third and lowest branch in Fig. 4 represents a solution with negligible combustion. Again, the middle branch corresponds to solutions with partial combustion and the upper one to solutions with full combustion.
Fig. 3. Temperature (a) and mass fraction profiles (b) for $\Delta = 8.8 \cdot 10^{-11}$.

Fig. 4. Bifurcation diagram: max. temperature vs. Peclet number ($\Delta = 8.8 \cdot 10^{-11}$).
We observe from Fig. 4 that there is a minimum Peclet number, \( Pe \approx 350 \), below which no solutions with combustion exist. This is qualitatively in agreement with experimental observations [1].

When following the upper branch in Fig. 4, the position of the reaction zone is moving from right to left for increasing \( Pe \). In the range \( 350 < Pe < 800 \) the combustion is not fully developed, although more than 70 percent of the reactant is consumed. From Fig. 5 we see that for \( Pe \) varying from about 800 up to 3000, solutions with full combustion exist, of which the reaction zone is located behind the jump discontinuity at \( x_i = 0.25 \). This clearly indicates its stabilizing effect on the location of the reaction zone.

![Graph showing mass fraction profiles](image_url)

**Fig. 5.** Mass fraction profiles of solutions at the upper branch for \( 815 < Pe < 3000 \) (Pe increasing from right to left).

## 4 Comparison with Two-Dimensional Problem

In this section we compare the one-dimensional steady-state solution with a numerical solution of a corresponding two-dimensional problem. The two-dimensional solution is obtained by transient simulation of the model including the flow equations, given by (1)–(5) and (8). The geometry of the upper half of the burner, measuring \( 0.08 \text{ m} \times 0.32 \text{ m} \), is shown in Fig. 1. The cooling at the boundary is modelled by (10).

The equations governing the flow (1)–(3) are discretized in space using a mixed finite element method on Raviart–Thomas elements of lowest order. For the spatial discretization of (4) and (8) we use a cell-centered finite volume scheme with upwinding for the convective part of the flux. Fully implicit time integration is used for the resulting system. The domain is resolved by a triangulated mesh. For other details of the computation we refer to [6].

At the inflow boundary \( \Gamma_1 \) we prescribe a constant mass flow rate \( \dot{m}_0 = 0.2 \text{ kg/m}^2\text{s} \), corresponding to \( Pe = 2680 \) and in case of complete combustion
to a flux density of released heat of $m_0h_0Q = 500$ kW/m$^2$. The fuel is ignited by an artificial heat source in region B near the discontinuity. The simulation is continued until a steady state is reached. The results of the simulation for the data of Tab. 1 are shown in Fig. 6. In Fig. 7 we compare the temperature and mass fraction distribution along the cooling boundary with the one-dimensional solution. We observe that the agreement here is very good. Because a finite thermal conductivity in the vertical direction leads to a non-uniform temperature distribution, the agreement at the axis of symmetry is only satisfactory.

![Fig. 6. Steady-state temperature (a) and mass fraction distribution (b).](image)

![Fig. 7. Comparison of 1D and 2D solution near cooling boundary: temperature (a), and mass fraction distribution (b).](image)
5 Conclusion

Using a numerical continuation method we computed the solution branches for a one-dimensional steady-state combustion problem. We showed that there is a minimum Peclet number below which no steady solutions with combustion exist. Furthermore, we showed that solutions with full combustion exist over a large range of mass flow rates (Peclet numbers), and that the jump in the porosity and cooling contributes to the stability of the combustion zone. Finally, comparing the one-dimensional solution with a solution of a corresponding two-dimensional problem, we found that the agreement along the cooling boundary is very good, and along the axis of symmetry satisfactory. The numerical bifurcation analysis of the one-dimensional problem can therefore be used as preparation for a computationally more expensive two-dimensional simulation.

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References