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Original Article

Mathematical model in the form of vorticity-stream function for porous premixed combustion

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Abstract

This paper proposes a mathematical model used to numerically simulate behaviors of the two-dimensional laminar premixed combustion in porous media. The governing equations proposed include vorticity-stream function equations. This set of the governing equations is non-dimensionalized and numerically solved based on finite difference algorithm. The rectangular computational domain filled with saturated porous media is subjected to premixed reactant mixture coming into the domain from the lateral wall. The top and bottom walls are insulated. The computation is conducted for half of the domain based on a symmetrical boundary with appropriate flow and thermal conditions. The proposed mathematical model is successfully validated against the published work. The computed results agree reasonably well with the previous work. The model is able to correctly describe physical behaviors of a premixed combustion in which preheat, reaction and post combustion zone are included.

Keywords: porous combustion, premixed combustion, mathematical model, vorticity-stream function

1. Introduction

Porous combustion has been used extensively in many important industrial applications due to many advantages over conventional or free space combustion. Combustion in porous media gives better energy recirculation, better flame stabilization with leaner flame stability limit, as well as higher combustion rate. Additionally, reduction of CO and NO_x can be achieved. A large number of numerical simulations have been carried out to study combustion in porous media for various different aspects such as properties of porous media, porous geometry, flame stabilization, formation of pollutants, flame structure, flame speed, conversion efficiency of the heat into radiation energy, etc. A mathematical model enables a numerical parametric study for applications that porous combustion is involved. A two-dimensional model of two different geometries of porous burner was developed to study the effect of multidimensionality on flames within the pore scale (Hackert *et al.*, 1999). The conservation equations solved include both gas-phase and solid-phase energy equations. A one-step global reaction mechanism for the complete combustion of fuel was utilized. The density was obtained from the ideal gas law. The conservation equations were solved using the alternating direction implicit (ADI) method, and the pressure field is solved using the SIMPLE algorithm (Patankar, 1980). Brenner *et al.* (2000) computed heat flow in porous media based on the pseudohomogeneous heat transfer and flow model which treated the solid and fluid phases as an artificial unique phase. The two-dimensional steady problem of a chemically reacting mixture gas including

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20 species was considered. The thermodynamic data was obtained from the CHEMKIN II database (Kee *et al.*, 1992). In 2001, experimental and numerical studies of porous combustions of H_2/Cl_2 for HCI synthesis were conducted (Wawrzinek *et al.*, 2001). The finite volume code was used for numerical investigation based on the local thermal equilibrium model. It was found that the flame speed and the adiabatic flame temperature were higher for the H_2/Cl_2 reaction compared to CH_4/air combustion. Effects of porous properties have also been investigated extensively (Barra *et al.*, 2003; Bobnovich *et al.*, 2007). These works focused on the flame stability analysis. The physical model of porous burner consists of two different-property layers. The interface between layers serves as a flame holder preventing flashback for a specific range (Barra *et al.*, 2003). Bubnovich *et al.* (2007) carried out the one-dimensional simulations on combustion behaviors within the two layers of different sizes of alumina balls. The Zeldovich's mechanism was utilized for modeling the formation of NO_x. Species fractions, Gas and solid Temperatures were solved using Newton's method while pressure was computed by the congradient method (Hockney and Eastwood, 1981).

A porous burner with integrated heat exchanger was modeled as a two-dimensional axially symmetric geometry (Malico *et al.*, 2000). The combustion reaction was described by the skeletal mechanism (Glarborg *et al.*, 1992). Non thermal equilibrium was considered between gas phase and solid phase. The chemical reaction rates and thermophysical properties were obtained using CHEMKIN II (Kee *et al.*, 1996). The SIMPLE method (Patankar, 1980) was employed to obtain the numerical solutions. Recently, a mathematical model accounting for turbulence effects was proposed to study one-dimensional combustion of the methane/air in a porous medium (de Lemos, 2006). The thermo-mechanical models based on the double-decomposition concept were employed (de Lemos, 2006 (2)). In this work, turbulence was predicted utilizing the macroscopic k-ε model.

In the present study, we propose a mathematical model based on vorticity stream function for studying a premixed combustion of methane taking place in porous media. To the best knowledge of the authors, the proposed model with the current approach has not been reported in the literature. The model is two-dimensional since it can be applied in situations that a lateral heat loss is considerable. This case has been found in many industrial burners that have small cross-sectional areas. To simplify a mathematical description of a real complex problem, the governing equations consisting of conservative equations are transformed into the vorticity-stream function formulation. This model allows substantially faster computations. Further, the set of equations is non-dimensionalized to facilitate the parametric analysis. The computations are carried out for a half domain for which the appropriate symmetric conditions are employed. This work sets the ground for further studies on the influences of related parameters, while offering generality to be applied in other relevant combustion problems.

2. Mathematical Formulation

Schematic configuration of the rectangular ($H \times L$) porous enclosure is depicted in Figure 1. Combustion of mixture gas is initialized at the right boundary while the top and bottom boundary are adiabatic.

2.1 Governing equations

In the present study, the porous medium is assumed to be homogeneous and thermally isotropic. Such a model can be used if the mass flow density, pore diameter, and porosity are not too high and if the heat transport properties and the temperature are not too low (Pickenacker, 1995). This model was successfully employed in the investigation of methane-air non-premixed combustion in porous media (Brenner *et al.*, 2000). The numerical calculations were consistent with experimental data. Further, the same model was used to numerically investigate porous combustion for HCI synthesis (Wawrzinek *et al.*, 2001) wherein the adiabatic flame temperature and flame speed were successfully carried out. Accordingly, the saturated fluid within the medium is considered in a local thermodynamic equilibrium (LTE) with the solid matrix (El-Refaee *et al.*, 1998; Nield and Bejan, 1999; Pakdee and Rattanadecho, 2011). The validity regime of local thermal equilibrium assumption has been established (Marafie and Vafai, 2001). The fluid flow is unsteady, laminar and incompressible. The pressure work and viscous dissipation are all assumed negligible. The thermophysical properties of the porous medium are taken to be constant. The Darcy-Forchhei mer- Brinkman model was used to represent the fluid transport within the porous medium (Marafie and Vafai, 2001; Nithiarasu *et al.*, 1996; Pakdee and Rattanadecho, 2009). The Brinkmann's and the Forchheimer's extensions treats the viscous stresses at the bounding walls and the non-linear drag effect due to the solid matrix respectively (Marafie and Vafai, 2001). Furthermore, the solid matrix is made of spherical particles, while the porosity and permeability of the medium are assumed to be uniform throughout the rectangular domain. We neglect body forces, the Soret and Dufour effects, and gas radiation. Using standard symbols, the transport equations involving stream function ψ, vorticity ω include

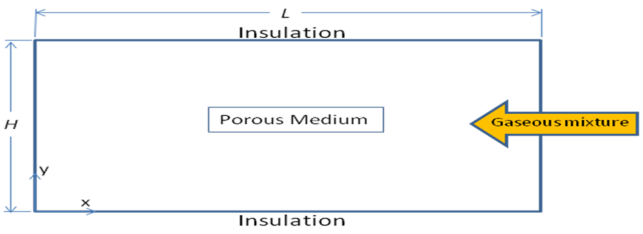

Figure 1. Schematic description of physical problem.

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}=-\omega$$

$$\frac{1}{\varepsilon}\frac{\partial\omega}{\partial t}+\frac{u}{\varepsilon^2}\frac{\partial\omega}{\partial x}+\frac{v}{\varepsilon^2}\frac{\partial\omega}{\partial y}=\frac{\upsilon}{\varepsilon}\left[\frac{\partial^2\omega}{\partial x^2}+\frac{\partial^2\omega}{\partial y^2}\right]-$$

$$\frac{\mu}{\rho_f\kappa}\omega-\frac{F}{\sqrt{\kappa}}|v|\omega+\frac{F}{\sqrt{\kappa}}\left(u\frac{\partial|v|}{\partial y}-v\frac{\partial|v|}{\partial x}\right)$$

$$\sigma\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}\right)=k\left[\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right]+\Delta h w^+$$

where Δh is the heat of reaction, and the heat capacity ratio,

$$\sigma=\frac{[\varepsilon(\rho c_p)_f+(1-\varepsilon)(\rho c_p)_s]}{(\rho c_p)_f}$$

where ε and υ are porosity and kinematics viscosity, respectively. The permeability κ and geometric F function are (Abdul-Rahim and Chamkha, 2001; Chamkha *et al.*, 2002)

$$\kappa=\frac{d_p^2\varepsilon^3}{175(1-\varepsilon)^2}$$

$$F=\frac{1.75(1-\varepsilon)}{d_p\varepsilon^3}$$

where d_p is the diameter of glass bead. The transport equations for fuel concentration C_f and air concentration C_a are given by

$$\varepsilon\frac{\partial C_f}{\partial t}+u\frac{\partial C_f}{\partial x}+v\frac{\partial C_f}{\partial y}=\rho D\left[\frac{\partial^2 C_f}{\partial x^2}+\frac{\partial^2 C_f}{\partial y^2}\right]+rw^+$$

$$\varepsilon\frac{\partial C_a}{\partial t}+u\frac{\partial C_a}{\partial x}+v\frac{\partial C_a}{\partial y}=\rho D\left[\frac{\partial^2 C_a}{\partial x^2}+\frac{\partial^2 C_a}{\partial y^2}\right]+w^+$$

where w^+ is the reaction rate and D is the mass diffusivity. The single-step global reaction for a complete combustion of methane is used.

2.2 Initial and boundary conditions

Premixed combustion of stoichiometric methane-air mixture is initialized at the right boundary which is considered the inflow boundary. At this boundary the imposed velocity field is $u = 6(y\text{-}y^2)$, $v = 0$. Using the definitions of stream function and vorticity in the two-dimensional plane $\left(\omega=\frac{\partial v}{\partial x}-\frac{\partial u}{\partial y}\right)$, the associated stream function and vorticity are $\psi=3y^2-2y^3$, $\omega=6-12y$ respectively. The top and bottom boundaries are stationary insulated walls in which

$$\frac{\partial T}{\partial y}=0,\ \psi=0 \text{ and as } \omega=-\frac{\partial u}{\partial y}, \text{ thus } \omega=-\frac{\partial^2\psi}{\partial y^2}.$$

At the outflow boundary where v-component velocity and its gradient $\left(\frac{\partial v}{\partial x}\right)$ are zero, and $\frac{\partial u}{\partial x}=0$ it can be shown that $\frac{\partial\psi}{\partial x}=0$ and $\omega=-\frac{\partial^2\psi}{\partial y^2}$.

At the centerline of the axisymmetric geometry, the associated variables are treated using symmetry conditions. Gradients of scalar variables as well as normal velocities are set to zero as.

$$\frac{\partial T}{\partial y}=\frac{\partial C_f}{\partial y}=\frac{\partial C_a}{\partial y}=0$$

Since v-component velocity is set to zero, we obtain $\frac{\partial\psi}{\partial x}=0$, and, again, from the definition of vorticity it turns out that $\omega=0$.

2.3 Non-dimensional governing equations

The governing equations are non-dimensionalized by the following parameters.

$$\bar{\psi}=\frac{\psi}{\alpha},\ \bar{\omega}=\frac{\omega L^2}{\alpha},$$

where thermal diffusivity $\alpha=\frac{k}{\rho c_p}$ and

$$\left.\begin{aligned}\bar{u}=\frac{u}{U},\ \bar{v}=\frac{v}{U},\ \bar{x}=\frac{x}{L},\ \bar{y}=\frac{y}{L}\\ \bar{T}=\frac{T}{T_{ref}},\ \bar{C}=\frac{C}{C_{ref}},\ \bar{t}=\frac{tU}{L}\end{aligned}\right\}$$

The non-dimensional equations are obtained as

$$\frac{\partial^2\bar{\psi}}{\partial\bar{x}^2}+\frac{\partial^2\bar{\psi}}{\partial\bar{y}^2}=-\bar{\omega}$$

$$\varepsilon\frac{\partial\bar{\omega}}{\partial\bar{t}}+\bar{u}\frac{\partial\bar{\omega}}{\partial\bar{x}}+\bar{v}\frac{\partial\bar{\omega}}{\partial\bar{y}}=\frac{\varepsilon}{\mathrm{Re}}\left[\frac{\partial^2\bar{\omega}}{\partial\bar{x}^2}+\frac{\partial^2\bar{\omega}}{\partial\bar{y}^2}\right]-\frac{\varepsilon^2}{\mathrm{Re}\,Da}\bar{\omega}-\frac{F}{\sqrt{Da}}|v|\bar{\omega}+$$

$$\frac{F}{\sqrt{Da}}\left(\bar{u}\frac{\partial|v|}{\partial\bar{y}}+\bar{v}\frac{\partial|v|}{\partial\bar{x}}\right)$$

$$\varepsilon\left(\frac{\partial\bar{C}_f}{\partial\bar{t}}\right)+\bar{u}\frac{\partial\bar{C}_f}{\partial\bar{x}}+\bar{v}\frac{\partial\bar{C}_f}{\partial\bar{y}}=\frac{1}{\mathrm{Re}\,Sc}\left[\frac{\partial^2\bar{C}_f}{\partial\bar{x}^2}+\frac{\partial^2\bar{C}_f}{\partial\bar{y}^2}\right]+\frac{L^2}{D\,\mathrm{Re}\,ScC_{ref}}rw^+$$

$$\varepsilon\left(\frac{\partial\bar{C}_a}{\partial\bar{t}}\right)+\bar{u}\frac{\partial\bar{C}_a}{\partial\bar{x}}+\bar{v}\frac{\partial\bar{C}_a}{\partial\bar{y}}=\frac{1}{\mathrm{Re}\,Sc}\left[\left(\frac{\partial^2\bar{C}_a}{\partial\bar{x}^2}+\frac{\partial^2\bar{C}_a}{\partial\bar{y}^2}\right)\right]+\frac{L^2}{D\,\mathrm{Re}\,ScC_{ref}}w^+$$

The global reaction rate for methane combustion is given by (Westbrook and Dryer, 1981)

$$w^{+} = 8.45\times10^{11}(Cref)^{2.8}(\overline{C_a})(\overline{C_f})^{1.8}e^{(-E/RT_{ref}\bar{T})}$$

Additionally, velocity components can be computed from

$$\frac{\partial\overline{\psi}}{\partial\overline{y}} = \overline{u} \quad \text{and} \quad -\frac{\partial\overline{\psi}}{\partial\overline{x}} = \overline{v}$$

Properties of methane and oxygen are considered for the present computations. The porous medium properties are based on the published data (Malico et al., 2000). Medium porosity and the Darcy number Da of 0.7 and 0.001 are used respectively. Reynolds number based on the length L, Re is 895. The Schmidt number Sc of CH_4 and O_2 of 0.73 and 0.83 are recommended by smooke and Giovangigli (1991).

2.4 Numerical approach

In the present study, the iterative finite difference method is used to solve the transient dimensionless governing equations subject to their corresponding initial and boundary conditions. Approximation of convective terms is based on an upwind finite differencing scheme, which correctly represents the directional influence of a disturbance. The relaxation method is used to solve for stable solutions. The velocity field is obtained by integration of the stream function. The computational domain was discretized into 30×110 uniform mesh. The grid dependency was determined. It was found that the peak temperature of the flame was lower by less than 2 % when the 30×220 mesh was used. The 30×110 mesh was found to be a good compromise between computational error and computational time.

3. Results and Discussion

The conditions for symmetric boundary are first examined. Computations of a full and half domain shown in Figure 2 reveal an accurate result. Half domain simulation greatly reduces both computational cost and required data storage.

In order to verify the accuracy of the proposed model, the results obtained by the present study is validated against the predicted solutions for premixed combustion in porous burners (Malico *et al.*, 2000). In this published work, the skeletal mechanisms were modeled to describe combustion which consists of 77 reactions and 26 species (Glarbog *et al.*, 1992). They validated their model with available experimental data (Trimis and Durst, 1996). The centerline temperatures were measured by using thermocouples that were passed through a ceramic pipe inside the ceramic foam. Comparision of the results represented by the centerline temperature is shown in Figure 3. The computed data in the present work are taken after the flame has stabilized as it propagates downstream. It was found that the solutions had good agreement with the previously published data (Malico *et al.*, 2000; Trimis and Durst, 1996). The predicted peak temperature and location of flame front agree well with the published data. However, a discrepancy near the right boundary is mainly attributed to the fact that the left wall is treated as a heat exchanger surface in the previous works (Malico *et al.*, 2000; Trimis and Durst, 1996). Further, the temperature difference between solid and gas is relatively larger in the preheat zone only. The gas temperature is higher than the solid temperature since the convective heat transport properties of the porous medium is not sufficiently high while the heat release from the solid matrix transfers to the mixture gas. Nevertheless, the overall prediction of temperature profile by the present mathematical model is reasonably accurate. All of the favorable comparisons lend confidence to the accuracy of the present numerical model.

Figures 4-6 show the time evolution of temperature fuel concentration and u-component velocity on two-dimensional domain. It is seen that flame front travels towards the left side of the domain corroding to the flow direction in Figure 6. Temperature is high in the inner area of the flame. The temperature gradient is high in the reaction region in which combustion occurs. In Figure 5, fuel is being consumed as the flame front propagates. The gradient of species concentration is high in the reaction region consistent to the area of high temperature gradient. These high gradients provide the driving forces for a self-sustaining flame

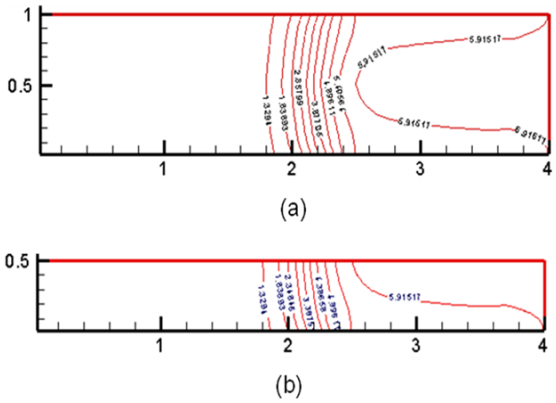

Figure 2. Temperature distributions on a two-dimensional axisymmetric geometry: (a) Full domain (b) half domain.

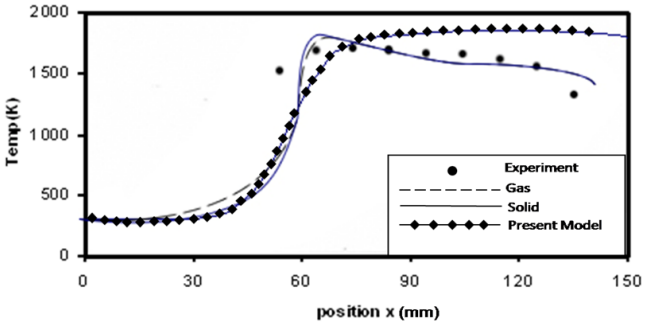

Figure 3. Comparison of the centerline temperature from the present model, the previous model (Malico *et al.*, 2000) and the experiment (Kee *et al.*, 1996)

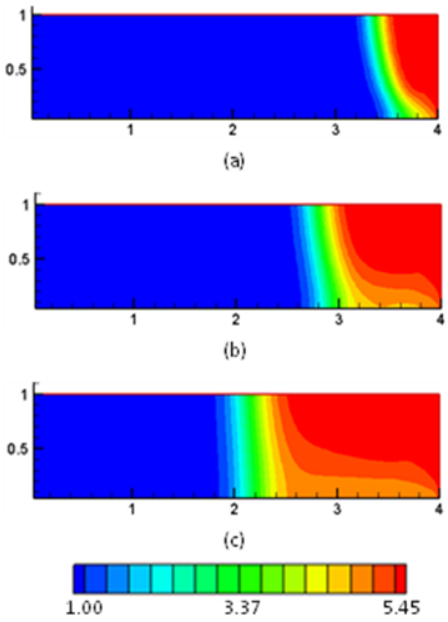

Figure 4. Temperature distributions at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

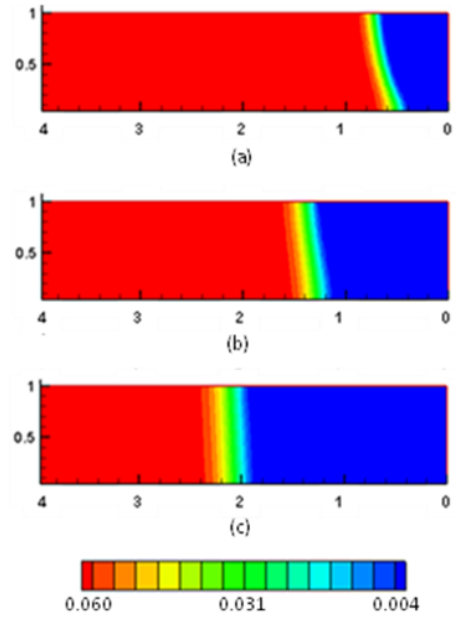

Figure 5. Distribution of fuel concentration at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

in which the porous structure recirculates heat from the post-flame to the pre-flame zone.

4. Conclusions

The simple mathematical model for a study of premixed combustion in porous media is developed. The accuracy of the model is successfully validated with the published

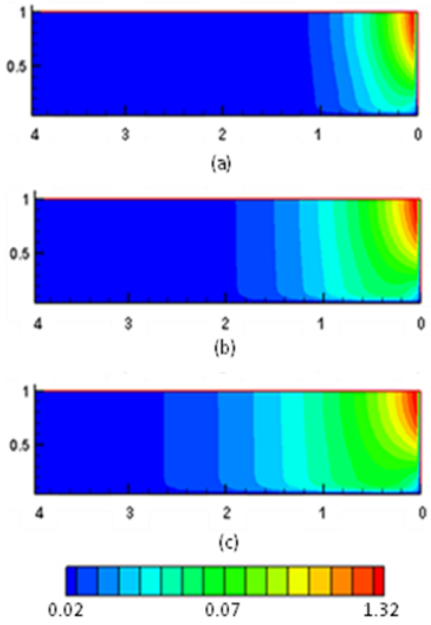

Figure 6. Distribution of u-component velocity at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

data. The governing equations are formulated in the form of vorticity-stream function. This set of the equations is non-dimensionalized and numerically solved based on finite difference algorithm. The computation is conducted for half of the domain based on the proposed symmetrical boundary with appropriate flow and thermal conditions. Results are demonstrated in terms of gas temperature, flow field and species concentration. The model is able to correctly describe physical behaviors of a premixed combustion in a porous medium. Future work will be the inclusion of complex chemical kinetics which enables prediction of pollutant formation rates.

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