Mathematical Model in the Form of Vorticity-Stream Function for Combustion in Porous Media

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Abstract

This paper proposes a mathematical model used to numerically simulate behaviours 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, 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 [1]. 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 [2]. G. Brenner et al. [3] 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 20 species was considered. The thermodynamic data was obtained from the CHEMKIN II database [4]. Effects of porous properties have also been investigated extensively [5-6]. 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 [5]. V. Bubnovich et. al. [6] 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 [7].

A porous burner with integrated heat exchanger was modeled [8] as a two-dimensional axially symmetric geometry. The combustion reaction was described by the skeletal mechanism [9]. Non thermal equilibrium was considered between Gas phase and solid phase. The chemical reaction rates and thermophysical properties were obtained using CHEMKIN II [10]. The SIMPLE method [2] was employed to obtain the numerical solutions. Recently, the mathematical model accounting turbulence effects was proposed to study one-dimensional combustion of the methane/air in a porous medium [11].The thermo-mechanical models based on the double-decomposition concept were employed [12]. In this work, Turbulence was predicted utilizing the macroscopic k-ε model.

In the present study, we propose the simple mathematical model for studying a premixed combustion of methane taking place in porous media. The model is two-dimensional since a lateral heat loss is considerable for 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.

2. Mathematical formulation

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

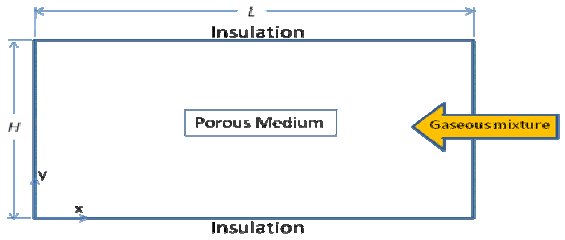

Fig. 1 Schematic description of physical problem.

2.1 Governing equations

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 [13]. Accordingly, the saturated fluid within the medium is considered in a local thermodynamic equilibrium (LTE) with the solid matrix [14 – 16]. The validity regime of local thermal equilibrium assumption has been established [17]. 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. However, the Boussinesq approximation takes into account of the effect of density variation on the buoyancy force. The Darcy-Forchheimer- Brinkman model was used to represent the fluid transport within the porous medium [17-19]. 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 [17]. 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 involve

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

$$\frac{1}{\varepsilon}\frac{\partial\omega}{\partial t}+\frac{u}{\varepsilon^2}\frac{\partial\omega}{\partial x}+\frac{v}{\varepsilon^2}\frac{\partial\omega}{\partial y}=\frac{\upsilon}{\varepsilon}\left[\frac{\partial^2\omega}{\partial x^2}+\frac{\partial^2\omega}{\partial y^2}\right]-\frac{\mu}{\rho_f\kappa}\omega$$
$$-\frac{F}{\sqrt{\kappa}}|v|\omega+\frac{F}{\sqrt{\kappa}}\left(u\frac{\partial|v|}{\partial y}-v\frac{\partial|v|}{\partial x}\right)$$

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

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, ν and β are porosity, kinematics viscosity and coefficient of thermal expansion of the water layer, respectively. The permeability κ and geometric F function are [20-21]

$$\kappa=\frac{d_p^2\varepsilon^3}{175(1-\varepsilon)^2}$$
$$F=\frac{1.75(1-\varepsilon)}{d_p\varepsilon^3}$$

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

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

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

where w^+ is the reaction rate. The single-step global reaction for a complete combustion of methane is used. The equations are non-dimensionalized by the following parameters.

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

The non-dimensional equations are obtained as

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

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

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

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

The global reaction rate for methane combustion is given by [22]

$$w^+ = 8.45 \times 10^{11} (Cref)^{1.8} (\bar{C}_a)(\bar{C}_f)^{1.8} e^{(-E/RT)}$$

Velocity components can be computed from

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

2.2. Initial and boundary condition

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 $u = 6(y - y^2), v = 0$. 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. The far-field condition is employed at the outflow boundary. At the centerline of the axisymmetric geometry, the associated variables are treated as

$$\frac{\partial T}{\partial y} = \frac{\partial C_f}{\partial y} = \frac{\partial C_a}{\partial y} = 0, \frac{\partial^2 \psi}{\partial y^2} = \frac{\partial u}{\partial y} = v = 0,$$

$$\frac{\partial v}{\partial x} = \omega$$

3. Results and Discussion

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

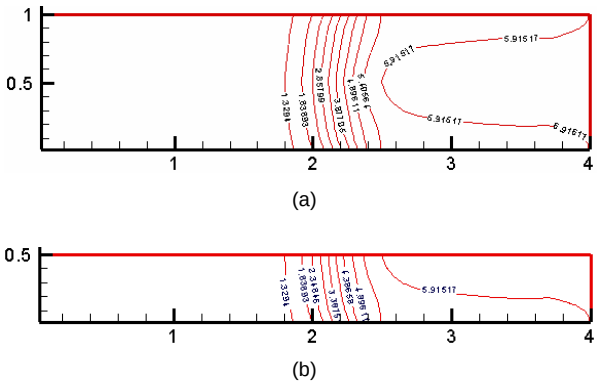

Fig. 2 Temperature distributions on a two-dimensional axisymmetric geometry: (a) Full domain (b) half domain.

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 [8]. In this published work, the skeletal mechanism [9] were modeled to describe combustion which consists of 77 reactions and 26 species. They validated their model with available experimental data. The comparing results represented by the centerline temperature are shown in Fig. 3 It was found that the solutions have good agreement with the previously published data. However, the causes of a discrepancy are due mainly to lack of detailed chemistry and the local thermal

equilibrium assumption used in our present work. It is seen that only in the preheat zone, the temperature difference between solid and gas is relatively large. The gas temperature is higher than the solid temperature. The heat release in the reaction zone transfers heat to the preheating zone while the convective heat transport properties of the porous medium is not sufficiently high. Nevertheless, the overall prediction of temperature profile by the present mathematical model is reasonably accurate.

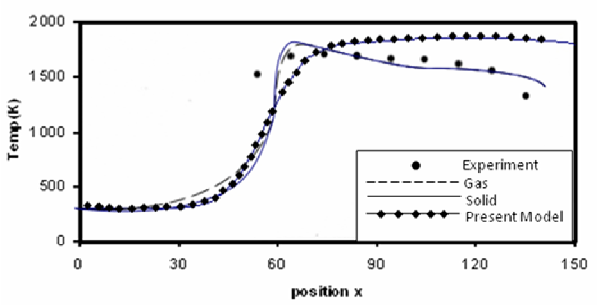

Fig. 3 Comparison of the centerline temperature from the present model, the previous model and experiment [8].

Figs.4 -6 shows 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 fig.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 fig.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.

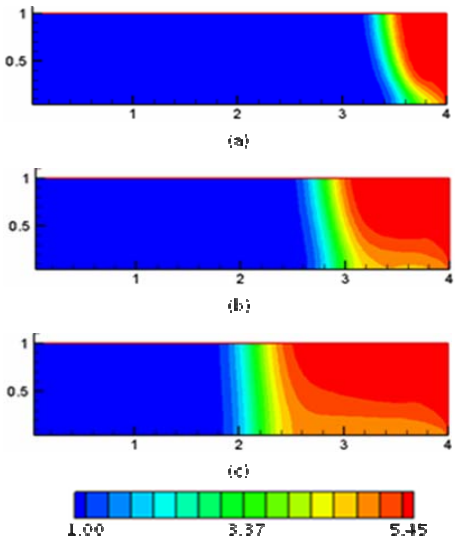

Fig. 4 Temperature distribution at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

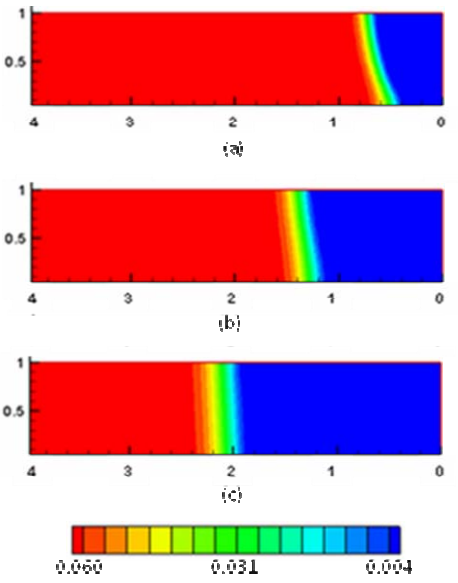

Fig. 5 Distribution of fuel concentration at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

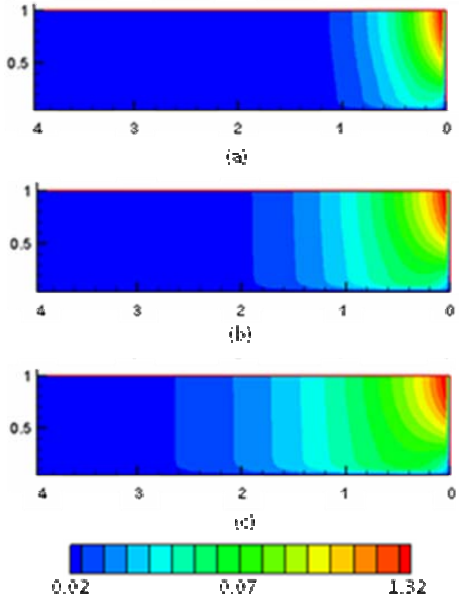

Fig. 6 Distribution of *u*-component velocity at different time, $\bar{t}$ of (a) 0.5, (b) 1.5 and (c) 3.0.

5. Conclusion

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 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.

7. References

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