A NUMERICAL STUDY OF COMBUSTION IN POROUS BURNER WITH A TWO-ENERGY EQUATION MODEL

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Abstract. *Premixed combustion inside a porous medium is an area currently under intense investigation due to the industry necessity of utilizing combustion chambers with high efficiency and low pollutants emissions. Applications of this technology in hydrogen production, oil recovery, and household heating combustion are being investigated by many groups of research. This technology is based on the control over the flame through the possibility of utilizing different porous materials inside the reactor in the preheat region and combustion region. The present work presents numerical simulations of combustion in porous media utilizing a two energy equation model. The reactor simulated has two different porous regions of different materials. A laminar two dimensional model is based on a macroscopic formulation of the transport equations. A global mechanism was utilized to model the chemical kinetics. Finite volume method is used with a boundary-fitted non-orthogonal coordinate system. The results present a comparison between the two-energy equation model, considering the difference between the temperatures of the solid and fluid phase, and a model with one energy equation making use of the local thermal equilibrium assumption.*

Keywords: *porous media burner, premixed flame, numerical simulation.*

1. INTRODUCTION

Porous media combustion devices can be classified into two categories, one in which the combustion is fully confined within the pores of the porous structure and the other one in which the combustion takes place over the surface of the porous matrix. The present work considers the first one which is receiving more attention of researchers due to the numerous advantages: burning of lean combustible mixtures, higher ranges of flame stability, lower pollutant formation, etc. (Howell et al. (1996)). Systems based on fluidized bed combustion, in-situ combustion for oil recovery, household heating combustion are just a few examples of such applications (Trimis and Durst (1996)).

Studies on macroscopic transport modeling of incompressible flows in porous media have been based on the volume-average methodology for either heat or mass transfer. The present paper follows the foregoing works and presents a two dimensional mathematical model for laminar pre-mixed flame combustion in porous media. Although in this work only one-dimensional plots are presented, computations of a two-dimensional laminar pre-mixed flame of methane/air were run. The numerical methodology employed is based on the control-volume approach with a boundary-fitted non-orthogonal coordinate system. The reactor consists of a two-region burner with a small pore size upstream and a large pore size downstream in order to achieve steady combustion in the porous media, the flame can be stabilized at the interface between the two different porosity blocks.

There are situations that the local thermal equilibrium hypothesis (Kaviany, 1995) is not applicable. These situations are characterized through a considerable difference between the solid phase temperature and the fluid phase temperature generally occurring due to the low rate of heat transfer between the two phases or high heat generation in one phase. These situations require a two-energy equation model: one to the fluid phase and another to the solid phase. Transient problems involving heat transfer between the two phases is another case that demands a two-energy equation model (Sathe *et al*., 1990; Malico *et al*., 2000; Hsu *et al*., 1993; Baek *et al*., 1989; Kaviany, 1995; Saito, 2006). The present study shows numerical simulations of an adiabatic reactor and the comparison between the two-energy equation model, considering the difference between the temperatures of the solid and fluid phase, and a model with one energy equation, making use of the local thermal equilibrium assumption.

2. MACROSCOPIC TRANSPORT EQUATIONS

2.1 Macroscopic continuity equation

$$\nabla.\mathbf{u}_D = 0 \tag{1}$$

where, $\mathbf{u}_D$ is the average surface velocity (also known as seepage, superficial, filter or Darcy velocity). Equation (1) represents the macroscopic continuity equation for an incompressible fluid.

2.2 Macroscopic momentum equation

$$\rho\left[\nabla\cdot\left(\frac{\mathbf{u}_\mathrm{D}\mathbf{u}_\mathrm{D}}{\phi}\right)\right]=-\nabla(\phi\langle p\rangle^f)+\mu\nabla^2\mathbf{u}_\mathrm{D}-\left[\frac{\mu\phi}{K}\mathbf{u}_\mathrm{D}+\frac{c_F\phi\rho|\mathbf{u}_\mathrm{D}|\mathbf{u}_\mathrm{D}}{\sqrt{K}}\right] \tag{2}$$

where, the last two terms in equation (2), represent the Darcy-Forchheimer contribution. The symbol K is the porous medium permeability, $c_F=0.55$ is the form drag coefficient (Forchheimer coefficient), $\langle p\rangle^f$ is the intrinsic (volume-averaged on fluid phase) pressure of the fluid, ρ is the fluid density and is a function of temperature, μ represents the fluid dynamic viscosity and ϕ is the porosity of the porous medium (Kaviany, 1995; Pedras, 2000).

2.3 Macroscopic Energy Equation

Considering the assumption of a pseudo-homogeneous medium wherein the solid and the fluid phases are treated as an artificial unique phase, the energy equation can be formulated as (Kaviany, 1995; Rocamora, 2001):

$$\left(\rho c_p\right)_f\nabla\cdot\left(\mathbf{u}_D\langle T\rangle^i\right)=\nabla\cdot\left\{\mathbf{K}_{eff}\cdot\nabla\langle T\rangle^i\right\}+\phi\Delta HS_{fu} \tag{3}$$

where, $\langle T\rangle^i$ is the averaged temperature for both the solid and the liquid according to the concept of local thermal equilibrium (Kaviany (1995), ΔH is the heat of combustion, S_{fu} is the rate of fuel consumption determined by a one-step Arrehnious rate equation, to be shown below, K_{eff} is the effective conductivity tensor given by,

$$\mathbf{K}_{eff}=\left\{\phi k_f+(1-\phi)\left[k_s+\frac{16\sigma\left(\langle T\rangle^i\right)^3}{3K_r}\right]\right\}\mathbf{I} \tag{4}$$

where, k_f and k_s are the thermal conductivities for the fluid and for the solid, K_r is the local Rosseland mean attenuation coeficient, σ is the Stefan-Boltzmann constant (Siegel *et al*., 2002).

2.4 Macroscopic Two-Energy Equations Model

$$\left(\rho c_p\right)_f\nabla\cdot\left(\mathbf{u}_D\langle T_f\rangle^f\right)=\nabla\cdot\left\{\mathbf{K}_{eff,f}\cdot\nabla\langle T_f\rangle^f\right\}+h_v\left(\langle T_s\rangle^s-\langle T_f\rangle^f\right)+\phi\Delta H\,S_{fu}{}^f \tag{5}$$

$$\nabla\cdot\left\{\mathbf{K}_{eff,s}\cdot\nabla\langle T_s\rangle^s\right\}-h_v\left(\langle T_s\rangle^s-\langle T_f\rangle^f\right)=0 \tag{6}$$

The equations (5) and (6) represent the energy equation for fluid and solid phase, respectively, where, $\langle T\rangle^f$ and $\langle T\rangle^s$ are the intrinsic volume average of the temperatures of the fluid phase and solid phase (Kaviany, 1995; Saito, 2006), ΔH is the heat of combustion, S_{fu} is the rate of fuel consumption determined by a one-step Arrehnious rate equation, to be shown below, h_v is the volumetric heat transfer coefficient and $\mathbf{K}_{eff,f}$ and $\mathbf{K}_{eff,s}$ are the effective conductivity tensors for the fluid and the solid phase, respectively, given by:

$$\mathbf{K}_{eff,f}=\lfloor\phi k_f\rfloor\mathbf{I} \tag{7}$$

$$\mathbf{K}_{eff,s}=(1-\phi)\left[k_s+\frac{16\sigma\left(\langle T_s\rangle\right)^3}{3K_r}\right]\mathbf{I} \tag{8}$$

The energy equations of the solid and fluid phases are coupled through the convection term and in this term there is the volumetric heat transfer coefficient (h_v). There are in the literature many empirical correlations that can be used to calculate the h_v . Fu *et al.* (1998) determined experimentally, through one inverse method, the h_v of five different ceramics with different porosities. The authors developed an empirical correlation to the convection heat transfer:

$$Nu_v = \frac{h_v {d_m}^2}{k_f} = C\,\mathrm{Re}^m \tag{9}$$

where: $h_v = a_v h$ and a_v is the specific surface area (i.e., area per unit volume). Kuwahara *et al.* (2001) present a numerical procedure, purely theoretical, applied to a structure composed of square rods representing the porous media. The empirical correlation provided by the numerical simulation is:

$$Nu = \frac{hD}{k_f} = \left(1 + \frac{4(1-\phi)}{\phi}\right) + \frac{1}{2}(1-\phi)^{1/2}\,{\mathrm{Re}_D}^{0.6}\,\mathrm{Pr}^{1/3}, \text{ where, } 0.2 < \phi < 0.9 \tag{10}$$

2.5 Macroscopic Mass Transport Equation

$$\nabla \cdot (\mathbf{u}_D \langle y_{fu} \rangle^f) = \nabla \cdot \mathbf{D}_{eff} \cdot \nabla(\phi \langle y_{fu} \rangle^f) + \phi S_{fu} \tag{11}$$

where, y_{fu} is the local mass fraction for the fuel. The effective mass diffusivity tensor, $\mathbf{D}_{eff}$, is defined as (Kaviany, 1995; Mesquita, 2003):

$$\mathbf{D}_{eff} = \frac{1}{\rho}\left(\frac{\mu_\phi}{Sc_\ell}\right)\mathbf{I} \tag{12}$$

where : Sc is the Schmidt number.

2.6 Combustion model

Premixed fuel and air enter the system which is characterized by two regions having different porosities. The region at the upstream end has a lower porosity than the one at the downstream end which works as a combustion chamber. The combustion reaction is assumed to occur in a single step according to the chemical equation:

$$CH_4 + 2(1+\Psi)(O_2 + 3.76N_2) \longrightarrow CO_2 + 2H_2O + 2\Psi O_2 + 7.52(1+\Psi)N_2 \tag{13}$$

where, ψ is the excess air in the reactant stream at the inlet of porous foam and is related to the equivalent ratio Φ by:

$$\Psi = \frac{1}{\Phi} - 1 \tag{14}$$

where,

$$\Phi = \frac{(y_{fu} / y_{ox})}{(y_{fu} / y_{ox})_{st}} \tag{15}$$

The ratio of fuel consumption is given by,

$$S_{fu} = \rho^2 A \langle y_{fu} \rangle^f \langle y_{Ox} \rangle^f \exp[-E_a / R\langle T \rangle\ ] \tag{16}$$

where, A is the pre-exponential factor, E_a is the activation energy and R is the universal gas constant. The gas density is updated using the ideal gas equation in the form,

$$\rho = P_0 / R^* \langle T \rangle^i \tag{17}$$

where, P_0 is a reference pressure, which is kept constant during the relaxation process, and $R^* = R/M$ and M is the gas molecular mass.

3. NUMERICAL MODEL

The governing equations were discretized using the finite volume procedure (Patankar, 1980) with a boundary-fitted non-orthogonal coordinate system. The SIMPLE algorithm for the pressure-velocity coupling was adopted to correct both the pressure and the velocity fields. The process starts with the solution of the two momentum equations. Then the velocity field is adjusted in order to satisfy the continuity principle. This adjustment is obtained by solving the pressure correction equation. A computational grid of 266x34 nodes is used in x- and y-direction.

The density is kept constant during the solution of the system of algebraic equations, but it is updated at each new interaction according to the ideal gas equation introduced bellow.

4. RESULTS AND DISCUSION

4.1 Geometry and coordinate system

Figure 4.1 presents the geometry of the porous media burner consisting of two distinct regions with different porosities and permeability. The gas mixture enters at the inflow boundary at the left, and the combustion products leave the burner at the outflow boundary at the right. The walls are impermeable and isolated. The porosity ϕ_1 is smaller than ϕ_2. All numerical parameters are found in Table 1, the activation energy and the pre-exponential factor were obtained from Malico (2001).

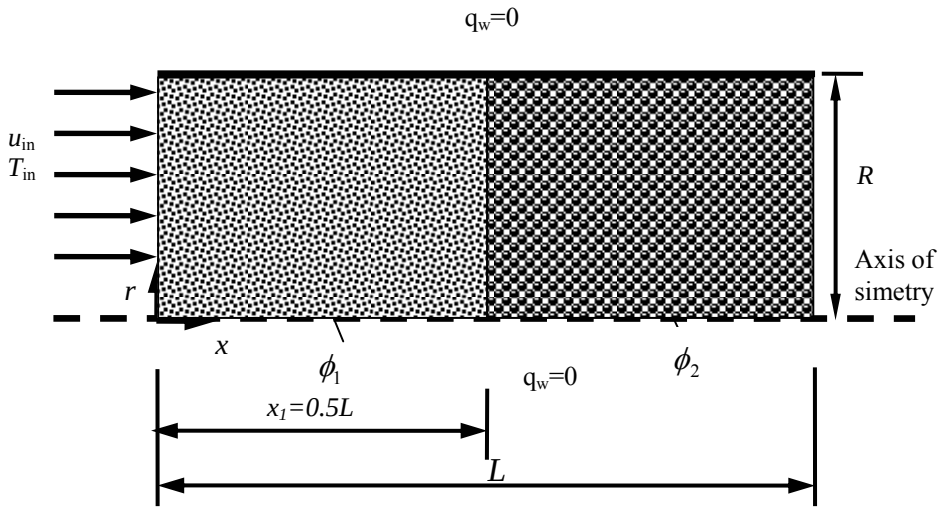

Figure 4.1 Geometry of a porous inert media burner and coordinate system.

4.2 Boundary conditions

The following boundary conditions are imposed on the solution:

$$\text{at x=0, u= } u_{in} \text{ , v=0, } \langle T \rangle^i = T_{in}, \ \langle y_{fu} \rangle^f = y_{fu,in}, \tag{18}$$

$$\text{at x=L, } \frac{\partial \langle T \rangle^i}{\partial x} = \frac{\partial \langle y_{fu} \rangle^f}{\partial x} = \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = 0 \tag{19}$$

where, u and v are the components of Darcy velocity vector in x and y. The non-slip condition for velocity is applied on both walls.

4.3 Temperature and fuel mass fraction profiles with different h_v correlations

The volumetric heat transfer coefficient (h_v), which is in the convective term, is responsible by the couple between the two energy equations and it is a source of great uncertainty in the literature. Many researchers investigated h_v in experiments involving or not combustion. In the figure 4.2 temperature profiles of the solid and fluid phase are presented, these profiles are related with the correlations obtained by Fu *et al.* (1998) and Kuwahara *et al.* (2001). The figure 4.2 presents also a temperature profile calculated with the one energy equation model and two temperature profiles, one to the fluid phase and other to the solid phase, obtained through the assumption of constant $h_v = 1x10^6$ $Wm^{-2}K^{-1}$. The curves show that only the two-energy equation model presents peak flame temperature, there is no peak of temperature at the curve obtained utilizing the one energy equation model.

At the beginning of the reaction zone, the characteristic time of the rate of reaction is small compared with the times of conduction, convection and radiation. The rate of change of the chemical enthalpy to the sensible enthalpy is greater than the local heat transfer rate and this provides the peak flame temperature. If the material employed had a high h_v, the peak flame temperature would be smaller or null. Increasing the h_v, makes with the peak flame temperature suffer a reduction. Approximating h_v to the infinity, the temperature profile of the solid phase approximates of the temperature profile of the fluid phase and both approximate of the temperature profile obtained with the one energy equation model (local thermal equilibrium assumption).

Table 1. Operating Conditions

Quantity	Value
Activation energy (J/mol) - Ea	$1.4x10^8$
Pre-exponential factor in reaction rate – A (m3/kg.s)	$1x10^{10}$
Length of the combustor – L (cm)	8
D (cm)	4
R (kJ/kmol.K)	8.3145
R* (kJ/kgK)	0.301
P_0 (kN/m2)	101.325
$y_{fuel,in}$	0.033784
T_{in} (K)	335
Matrix 1:	
K_1 (m2)	$1.477x10^{-8}$
ϕ_1	0,86
Matrix 2:	
K_2 (m2)	$3.698x10^{-7}$
ϕ_2	0,90

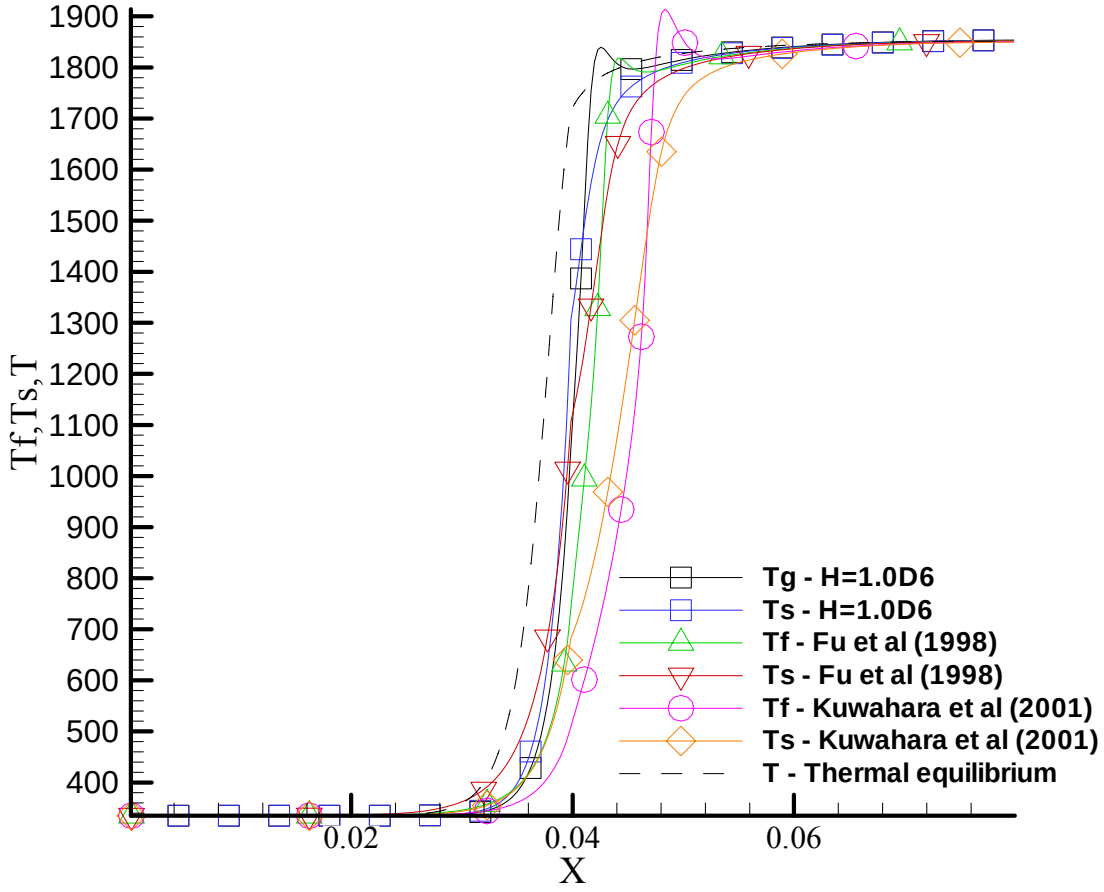

Figure 4.2: Temperatures profiles obtained utilizing different correlations to h_v : Kuwahara et al. (2001), Fu et al. (1998), constant h_v and the comparison with the model considering the assumption of local thermal equilibrium; y/H=0.5.

The figure 4.3 presents the fuel mass fraction profiles calculated with the one energy equation model and the two-energy equation model. The figure presents also the profiles calculated with different h_v correlations. The correlations adopted have a strong influence in the flame position as it is possible to see by the fuel consumption profiles in the figure 4.3.

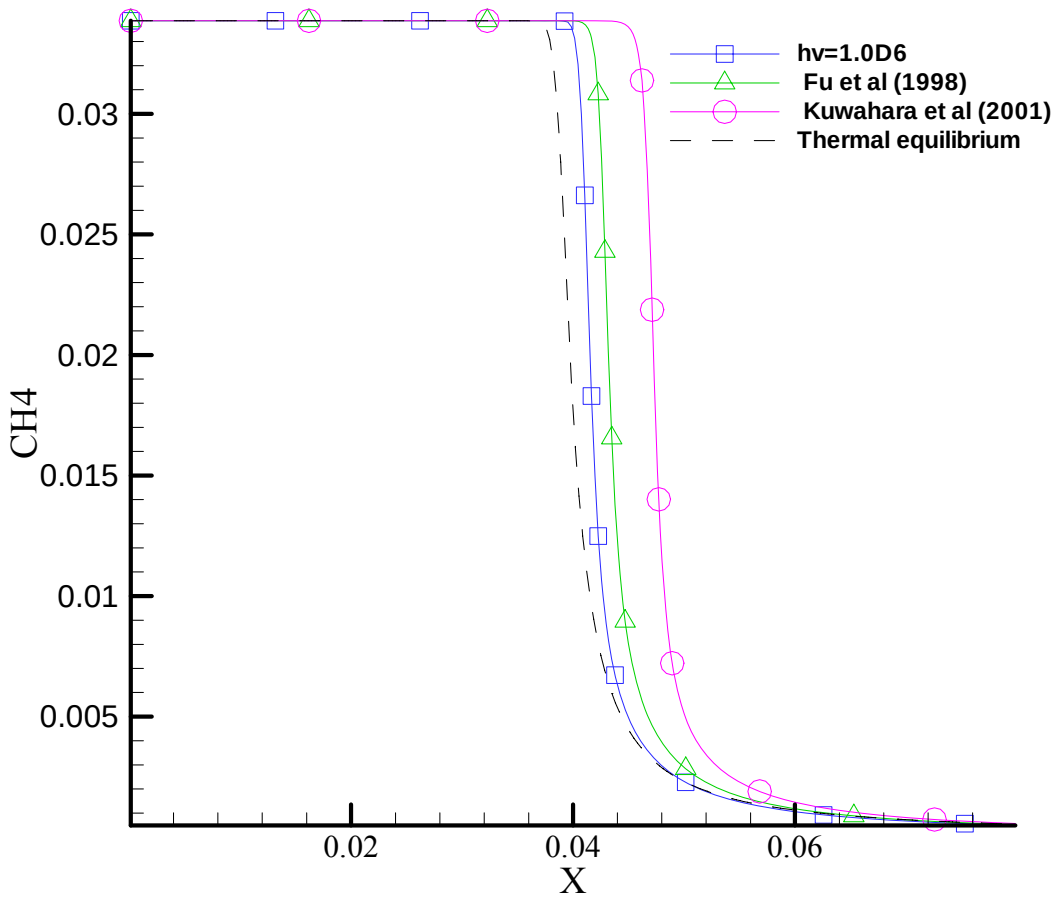

Figure 4.3: Fuel mass fraction profiles obtained utilizing different correlations to h_v : Kuwahara et al. (2001), Fu et al. (1998), constant h_v , and the comparison with the model considering the assumption of local thermal equilibrium; y/H=0.5.

5. CONCLUSION

The two-energy equation model was investigated. The model introduce an additional couple and the volumetric heat transfer coefficient become a new thermophysical property that needs to be treated, consequently, it is a new source of uncertainty. The results obtained with different h_v correlations presented different temperature and fuel mass fraction profiles. Similarly, the uncertainty in relation to h_v was reported by Malico (2001). Different correlations to h_v provided different curves of fuel consumption and provide different forecasts of pollutant emissions as will be presented in a subsequent paper.

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