Numerical Study of the Effects of Porous Burner Parameters on Combustion and Pollutants Formation

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Abstract— **In recent years, more attention has been focused on the use of porous materials to enhance the efficiency of combustion systems and to reduce the emission of pollutants. This is because combustion in inert porous media offers an interesting and promising route towards burner with high-power density, high-power dynamic range, and very low emission of pollutants such as NO_x and CO. This work reports one-dimensional combustion in a porous burner using three combustion models: GRI 3.0, GRI 1.2, skeletal mechanism. We conclude that skeletal mechanism has a good agreement with GRI 3.0 and it costs less. At first, we present a numerical study which shows the effects of these models on temperature, species and pollutant emissions. Then, we investigate the effects of volumetric heat transfer and emissivity coefficient and porosity on combustion and pollutions. It was concluded that NO and CO emission depend mainly on the volumetric and emissivity coefficient. When volumetric heat transfer decreased, the difference between gas and solid temperature reduced, therewith NO formation noticeably decreased whereas CO emission didn't change sensible. On the other hand, the flame peak temperature is reduced with the reduction of the solid emissivity coefficient. This important conclusion means that NO and CO emission and velocity increases. Also gas and solid temperature increase and vice versa. The other parameter is Porosity. Increasing in porosity of burner resulted in decreasing gas and solid temperature and subsequently NO and CO emission decreased sensible. Porosity has effected on velocity, too. As porosity decreased, velocity increased. Emissivity effects on the rate of heat flux which issue from burner. As the emissivity increased the efficiency of burner arose. So these parameters have important roles in decreasing the emission especially on No emission because it has more depend on temperature. In addition the resulted gas and solid temperatures were compared with reported measurements of center line temperature in a cylindrical porous burner. The good agreement with experimental observation upholds that the numerical model is a perfect tool to investigate combustion and pollutants formation in porous media.**

Keywords—**Emissivity Coefficient, Porosity, Porous burner, Volumetric Heat Transfer**

I. INTRODUCTION

Over the past 30 years, our understanding of combustion in porous media has increased substantially [1]–[2]. Development of porous burners has been encouraged by lower emission standards as well as the advantages these burners offer such as fuel flexibility, high-power density, high-power dynamic range and also the ability to operate at low equivalence ratios, and effective flame speeds greater than the laminar flame speed [3]–[5]. This is due to the high heat capacity, high conductivity and high emissivity of the solid matrix in comparison to a gas. In a porous burner, the porous matrix re-circulates heat from the post-flame to the pre-flame zone through solid-to-solid radiation and conduction leading to excess enthalpy flames [5]–[7]. This regenerative internal heat feedback mechanism results in several interesting characteristics relative to a free-burning flame, namely higher burning speeds, extension of the lean flammability limit, low emission of pollutants and the ability to burn fuels that have a low energy content. Also, inert porous media combustors may offer high compact very small scale sizes, which correspond to the desired characteristics of industrial applications or household heating combustion.

Development and optimization design of advanced combustion systems which meet pollutant emission standards and maintain or increase productivity will require mathematical modelling of the systems. The reduction in time between a system concept and commercialization and the increase in the cost of testing will demand a greater reliance on mathematical models to simulate the systems and reduce the cost and time to develop a product. Thus, models with varying degrees of sophistication have been recently developed and applied to the problem of predicting flame speeds, temperature and concentration profiles and radiative efficiency of combustion within porous media. A detailed review of modelling combustion in porous media can be found in Howel et al. (1996).

An early analysis was completed by Echigo (1982) to investigate the ability of converting some of the enthalpy of a non-reacting hot gas for radiative transfer from a porous medium through which the gas is flowing. The Echigo and co-workers (Echigo et al., 1986; Yoshizawa et al., 1988; Echigo, 1991) provided a rigorous model for multi-mode heat transfer, Arrhenius-type one-step reaction kinetics and exact solution for radiative transfer in the absorbing/emitting medium. However, because few data were available at the time of this work on thermo physical or transport properties in these systems, they made various simplifying assumptions and choices of property values. A single-step mechanism was used for methane combustion, so that multiple species equations could be dispensed. And it was assumed that the burner could be divided into three regions. an upstream region where no reactions occur, so that the gas/solid temperature were constant; a combustion zone, where the one-step combustion reaction goes to completion; and an exit zone, where the gases leaving the combustion zone again undergo

Manuscript submission April, 21, 2008
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no further reaction. Based on these assumptions, temperature profiles in the gas were predicted.

Chen et al. (1987) applied the energy and species equations to model porous medium burners. Noting the deficiency of one-step kinetics in the Yoshizawa et al. (1988) analysis, a multi-step mechanism for methane combustion was used in the model, based on the reaction set from the code CHEMKIN by Kee et al. (1980) which includes 17 species and 55 reactions. Parametric variations of the thermal conductivity of the solid, volumetric heat transfer coefficient and radiative properties were carried out to determine their effect on flame speed and temperature profiles.

In 1991, Tong and co-workers surveyed application of porous material in the burner structure [8]. They supposed one dimensional system and using Spherical harmonic method in calculating of radiation flux. They found that for maximum radiation outlet flux, they should use from porous layer with high thickness. They simulate the combustion phenomena with a source of steady heat generation in the porous media.

Hsu et al. (Hsu et al., 1993 and Hsu and Matthews, 1993) extended Chen's model to include the Zeldovich mechanism (3 reactions and two additional species) for No chemistry, and experimental values for thermal conductivity and radiative extinction coefficient that were unavailable to Chen (1988). In addition, a two-region burner with a small-pore size upstream section and large-pore downstream section was modeled. Hsu compared his modelling results with experimental data gathered on two-region porous media burners made of partially stabilized zirconia of various pores size. The model was accurate in predicting the maximum flame speeds sustainable within the burner (blow-off limit); the minimum equivalence ratio for sustainable combustion; the trends of flame speed with pore diameter and equivalence ratio and the measured emissions of CO, CO2 and NO. The model couldn't, however, predict the minimum sustainable flame speeds in the burner.

Lee et al. (1996) had experimentally and numerically investigated the combustion of premixed propane-air mixture inside a honeycomb ceramic. They used the one-dimensional flame structure model and a one-step reaction mechanism. They obtained the upstream and downstream solutions corresponding to each upper and lower solution. These are correspondent with the experimental results.

Viskanta and Gore [2] performed a numerical study using cordierite with 26 pores per centimeter (ppc) in the upstream section and cordierite LS-2 (4 ppc) in the downstream section. The total burner length was approximately 2.5 cm, including both the upstream and downstream layer, and the firing rates varied from 236 (kW/m^2) to 394 (kW/m^2) at an equivalence ratio of 0.9 for a methane/air mixture. They used the experimentally observed flame location to predict the temperatures and radiant output. Viskanta and Gore's results show that a larger heat transfer coefficient results in a higher peak solid temperature, which promoted higher radiative flux from the high temperature zone, but did not significantly affect the maximum gas temperature. In addition, increasing conductivity in the downstream section results in decreasing in solid temperature.

Kulkarni and Peck [9] modeled a 5 cm long two section burner. They determined the effect of porosity, length, radiation extinction coefficient, and albedo on radiant output from the burner. They concluded that the upstream layer should be of lower porosity, shorter length, and higher optical thickness (product of extinction coefficient and length) than the downstream layer and that the upstream layer should be scattering and the downstream non-scattering in order to maximize radiant output.

In 2000, Brenner and co-workers assumed two dimensional systems and solve the governing equations for combustion but they did not use any model for radiation [10].

In 2003, Talukdar and co-workers studied porous burner in two conditions, steady state and transient state, in the two dimensional system [11]. In this study, the effect of radiation diffusion to surrounding was considered. They used Collapsed Dimension method to specify radiation flux inert porous burner [12].

The purpose of the present work is to develop a mathematical model for fluid flow, combustion and heat transfer in porous media via development of the PREMIX code which is used for modeling steady laminar one-dimensional premixed flames.

In this paper, we modeled one- dimensional combustion and heat transfer of methane/air fuel in a two-region burner with a small-pore size upstream section and large-pore downstream section. Three mechanisms for the methane/air fuel combustion were used in this model. First Mechanism is GRI-3.0 which includes 77 species and 227 reactions [13]. Second mechanism is GRI-1.2 that includes 32 species and 177 reactions. Third mechanism is Skeletal mechanism. This Skeletal mechanism was developed by Glarborg et al. [14]. It is derived from the full reaction mechanism through sensitivity analysis and rate of production analysis of perfectly stirred reactor calculations covering the range of interest. This Skeletal mechanism comprises 26 species and 77 elemental reactions. The purpose of this skeletal mechanism is to provide a good description of methane oxidation including nitrogen chemistry at high temperature (T>1500K) and not excessively fuel-rich conditions.

Compared to the full mechanism, the most important simplification of the Skeletal model is the exclusion of C2-hydrocarbon chemistry. However, the most important reaction steps for methane oxidation and nitrogen chemistry are retained in the skeletal scheme.

We investigated the effects of volumetric heat transfer, emissivity coefficient and porosity on the temperature profiles and emission of Co and No in a porous burner. In addition, the predicted gas and solid temperatures were compared with experimental observation. The focus of this paper is on the predicted pollutants formation and their comparison with experiments.

The good agreement with experimental observations suggests that using this developed PREMIX code is an excellent tool to investigate the different gas fuel combustion and pollutants formation in porous media. Also this method costs low prices.

II. Numerical Method

The problem considered in the present study is a one-dimensional methane/air fuel combustion process within a porous burner. The model has been adapted from that described in Zhou and Pereira [15] and Henneke and Ellzey [16] for two sections of porous media.

The present modelling of combustion within porous media has made the following principal assumptions:
(1) The flame structure and heat transfer mechanism are one-dimensional.
(2) Potential catalytic effects of the high temperature solid are negligible.
(3) The Dofour, Soret, 'bulk' viscosity and body forces are negligible.
(4) The flow speed is sufficiently low that the process is isobaric.
(5) The mixture gas is non radiating.
(6) Compressibility effects are neglected

Based upon the above assumptions, the flame can be assumed to be one-dimensional and solved by using adiabatic laminar flame theory. The one-dimensional laminar flame PREMIX code [17] was modified for current use. This code allows the use of three mechanism detailed chemical kinetics [18] and use of the TRANFIT subroutine [19] for accurate determination of the transport properties of the gas. We made some changes in this code to solve this problem.

These changes include these items:

1- Adding porous material's properties and calculating the coefficient of radiation heat transfer.

2- Adding radiative equation of porous media in governing equations

3- Adding energy conservation equation of solid phase

4- Adding porosity in governing equations and term of convection heat transfer in gas and solid phase equations

5- Changing in boundary conditions

A. Burner geometry

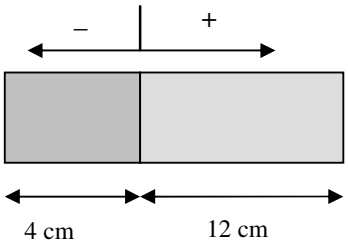

Figure 1 Porous burner schematic

B. Governing equations

The following conservation equations for mass, gas energy, solid energy, and gas species are solved:

$$\frac{\partial(\rho_g \phi)}{\partial t} + \frac{\partial(\rho_g u_g \phi)}{\partial x} = 0 \tag{1}$$

$$\rho_g \phi\ c_{p,g}\frac{\partial T_g}{\partial t} + \rho_g \phi\ u_g c_{p,g}\frac{\partial T_g}{\partial x} - \phi\ k_g \frac{\partial^2 T_g}{\partial x^2} + (1-\phi)\ h_v(T_g - T_s) + \phi\sum_{k=1}^{K}\rho_g Y_k V_k c_{p,k}\frac{\partial T}{\partial x} + \phi\sum_{k=1}^{K}\dot{\omega}_k h_k W_k = 0 \tag{2}$$

$$\rho_s \phi\ \ c_{p,s}\frac{\partial T_s}{\partial t} + (1-\phi)k_s \frac{\partial^2 T_s}{\partial x^2} - (1-\phi)h_v(T_s - T_g) - \frac{dq_n}{dx} = 0 \tag{3}$$

$$\rho_g \phi \frac{\partial Y_k}{\partial t} + \rho_g \phi\ \ u_g \frac{\partial Y_k}{\partial x} + \frac{\partial}{\partial x}\left(\rho_g \phi Y_k V_k\right) - \phi\,\dot{\omega}_k W_k = 0 \quad (k = 1,\ldots,K) \tag{4}$$

The radiation equation calculates from two-flux model [20]:

$$\frac{dq^+}{dx} = -2\sigma_a q^+ - 2b\varepsilon\ \ q^+ + 2\sigma_a \sigma\ \ T_s^4 + 2b\varepsilon\ \ q^- \tag{5}$$

$$-\frac{dq^-}{dx} = -2\sigma_a q^- - 2b\varepsilon\ \ q^- + 2\sigma_a \sigma\ \ T_s^4 + 2b\varepsilon\ \ q^+ \tag{6}$$

$$\frac{dq_n}{dx} = \frac{dq^+}{dx} - \frac{dq^-}{dx} \tag{7}$$

Convection was included by solving separate energy equations for the solid and the gas and coupling them through a convective heat transfer coefficient. The energy equation for the gas does not include radiation terms and the energy equation for the solid does not include energy liberation (reaction) terms.

Gas phase thermo chemical and transport properties are obtained from the CHEMKIN [17] and TRANFIT [18] packages. All simulations are conducted for methane/air mixtures. The GRI 1.2 chemical kinetics mechanism [21]–[22] with 32 species and 177 reactions, GRI 3.0 [13] with 77 species and 227 reactions and Skeletal mechanism [14] with 26 species and 77 elemental reactions is used to represent the chemistry.

C. Boundary conditions

The conditions specified at the inlet are the temperature and mass fraction of methane/air fuel and two below equations:

At the inlet:

$$\begin{cases} \dot{m} c_{p,g}(T_{i,g} - T_g) = -k_g \dfrac{dT_g}{dx} & at \quad x = 0 \\ (1-\phi)\ \left[h_v(T_{i,g} - T_s) + \sigma\varepsilon\left(T_{i,g}^4 - T_s^4\right)\right] = -k_s \dfrac{dT_s}{dx} & at \quad x = 0 \\ T = T_{in} \\ Y = Y_{k,in} \end{cases} \tag{8}$$

The conditions specified at the outlet are the temperature and mass fraction of methane/air fuel and one below equation:

At the outlet:

$$\begin{cases} \dfrac{dT_g}{dx}=0 & at \quad x=L \\ (1-\phi)\left[h_o\left(T_{o,g}-T_s\right)+\sigma\varepsilon\left(T_{o,sur}^4-T_s^4\right)\right]=-k_s\dfrac{dT_s}{dx} & at \quad x=L \\ \dfrac{dY_k}{dx}=0 \end{cases} \quad (9)$$

D. Solution method

The governing equations were solved with the damped Newton scheme used by modified PREMIX code. The number of grid began with 6 and continued to 200 grids.

The run time is very dependent on initial guess. Typically 2-20 minutes is needed in a Pentium 4 computer for cases started with good initial guesses.

In some cases, the problem takes several hours to reach converged solution. For example, to solve this problem with GRI 3.0 mechanism, it takes 1 hour. For all cases, a relative convergence of 10^{-5} was specified, which corresponds to four significant digits in the results. The absolute convergence was 10^{-9}. The grid effects on the solutions were examined by increasing the number of grid points after initial solution until the results changed no longer in a specified tolerance.

III. RESULT AND DISCUSSION

Fig. 2 displays the gas temperature profiles in porous media with stoichiometric and power 5000 kw/m^2. As this Figure shows, GRI 1.2 has a good agreement with GRI 3.0. These results have a good agreement with that described in Zhou and Pereira [15] and Henneke and Ellzey [16] for two sections of porous media.

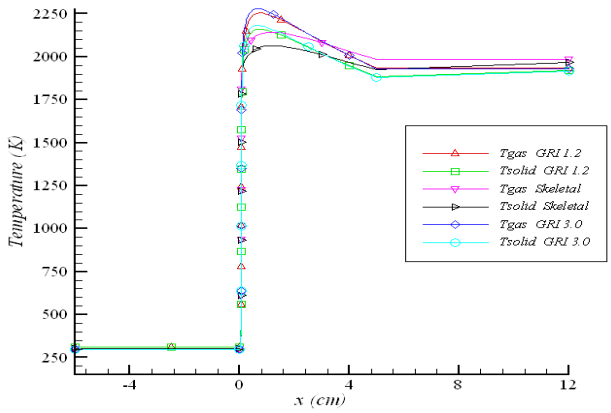

Figure 2 Temperature profiles for stoichiometric combustion and 5000 kw/m^2 power

Fig. 2 displays the temperature profiles of gas phase and solid matrix in stoichiometric and power 5000 kw/m^2. The temperature for gas and solid at inlet and outlet of burner is almost the same, but the difference at the flame front is evident. This shows that the assumption of the same temperature of solid and gas within porous media is not correct.

As it is obvious in Fig. 3, which shows CO profiles toward distance (x), the maximum of CO was produced at the flame front and it decreased in downstream again. Fig. 4 shows the CO_2 profiles toward distance (x). It exhibits that production of CO_2 is depends on the temperature. As the temperature increased the concentration of CO_2 increased significantly.

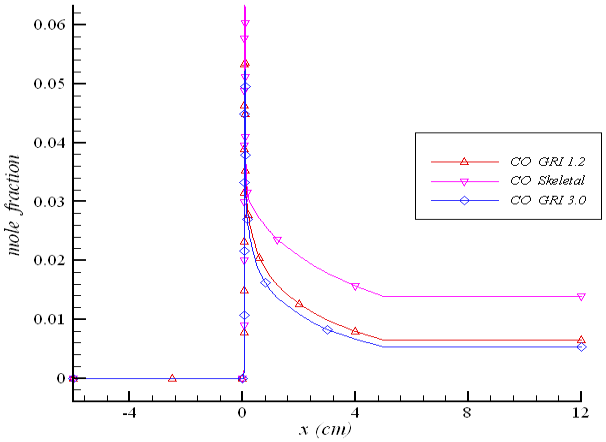

Figure 3 Emission of CO for different reaction mechanism with stoichiometric combustion in 5000 kw/m^2 power

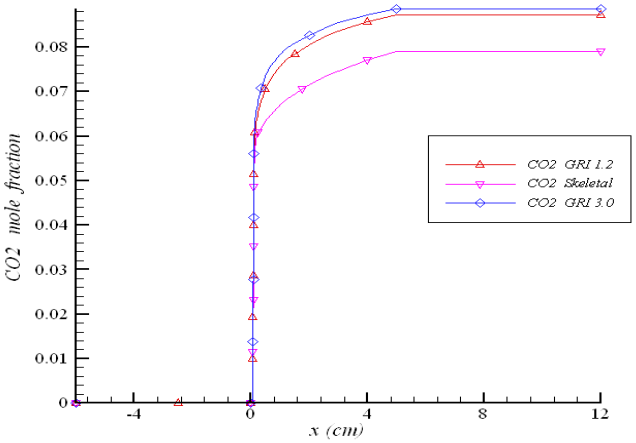

Figure 4 Emission of CO_2 for different reaction mechanism with stoichiometric combustion in 5000 kw/m^2 power

Fig. 5 shows NO profiles. Most of NO was produced at the flame front. It is obvious that temperature effects the production of NO considerably. From figure 2, GRI 3.0 and Skeletal mechanism have a little difference in estimating of temperatures profiles.

This little variance make a greatly difference in NO production. For Skeletal mechanism, the pick temperature is 2143 K, the exit NO is 0.00034, for GRI 3.0 mechanism the pick temperature is 2280 K, and the exit NO is 0.00020.

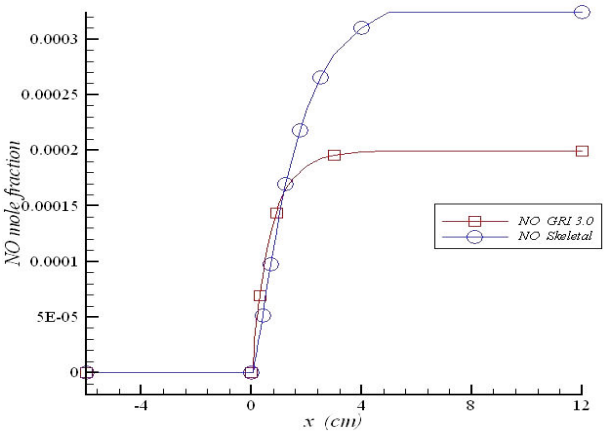

Figure 5 Emission of NO for stoichiometric combustion and 5000 kw/m^2 power

The effect of volumetric heat transfer on temperature profiles are shown in Fig. 6. GRI 3.0 reaction mechanism used in volumetric heat transfer effected on the difference between gas and solid temperature. As the volumetric heat transfer increased, the temperature of solid and gas got closely together.

It can be explained by this fact that high volumetric heat transfer can cause more heat transfer between gas and solid, so their temperature became closely together. The other effect is on the gas temperature. By increasing the volumetric heat transfer the gas temperature decreased slowly.

The effect of emissivity on temperature profile was shown in Fig. 7. This picture shows that when emissivity decreased the temperature of gas and solid increased considerably. It is because of by decreasing the emissivity factor the heat transfer to surrounding decreases. So the heat remains in the porous burner and increases the temperature. On the other hand, increasing in the temperature causes increasing the emission of NO and CO rapidly.

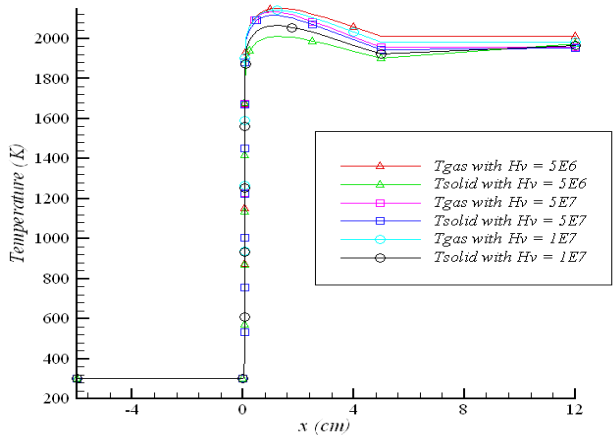

Figure 6 Temperature profiles for different volumetric heat transfer

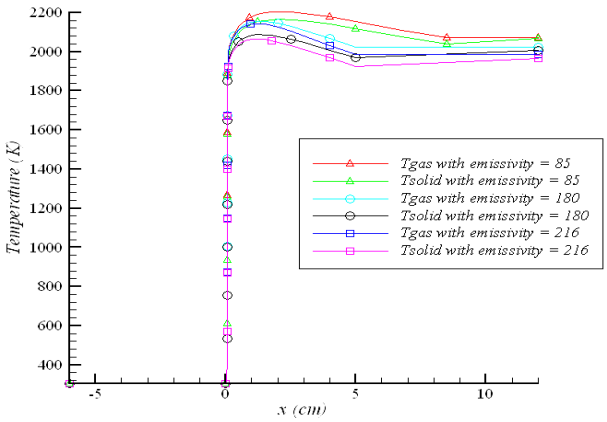

Figure 7 Temperature profiles for different emissivity

Fig. 8 expresses the temperature profiles with different porosity. Porosity has important effect on the temperature. As the porosity decreased the peak of temperature increased significantly and the temperature of the outlet gas increased, too.

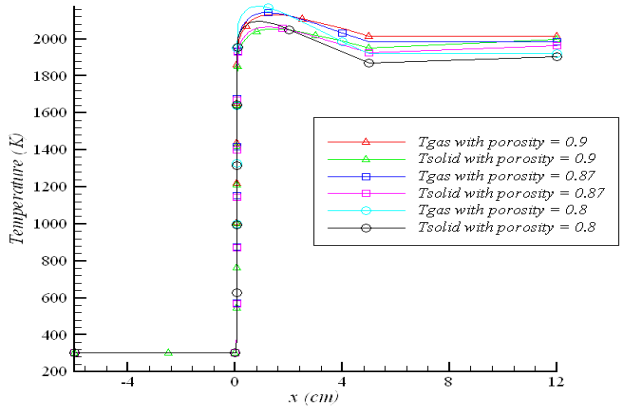

Figure 8 Temperature profiles for different porosity

This can explain that some characteristics of porous media such as high emissivity make a good heat transfer with surrounding and removing the heat which produces from combustion. This is an important parameter for decreasing emissions.

ACKNOWLEDGMENT

This work was supported by Office of Research of Sahand University of Technology and I would like to thank the head of this office.

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