Numerical Analysis of Turbulent Diffusion Combustion in Porous Media

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ABSTRACT

Turbulent methane-air combustion in porous burner is numerically investigated. Several computed field variables considered include temperature, stream function, and species mass fractions. The one-step reaction considered consists of 4 species. The analysis was done through a comparison with the gas-phase combustion. Porous combustion was found to level down the peak temperature while giving more uniform distribution throughout the domain. The porous combustion as in a burner is proved to provide wider flame stability limits and can hold an extended range of firing capabilities due to an energy recirculation.

1. Introduction

The 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. These features lead to higher turndown ratio (Kamal,
M.M. and Mohamad, 2005). Additionally, reduction of CO and NO\textsubscript{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. While premixed combustion in porous media has been extensively studied, diffusion or non-premixed combustion has never been studied in detail.

Porous medium burners are characterized by higher burning rates increased flame stabilization and minimized emissions. On account of these qualities, there are many fields of application for porous media combustion. In order to optimize the combustion process in porous media to promptly adapt porous materials and burner geometries to new applications, numerical simulations are necessary. Therefore the main purpose of this study is to carry out a numerical investigation of diffusion combustion in porous media.

2. Problem Description

The present work examines chemical species mixing and diffusion combustion of a gaseous fuel. A cylindrical combustor burning methane (CH\textsubscript{4}) in air is studied using the finite-rate chemistry model in FLUENT, a computational fluid dynamics (CFD) code (Fluent, 2003). The cylindrical combustor considered in this study is shown in Figure 1 for a two-dimensional configuration. The flame considered is a turbulent diffusion flame. A small nozzle in the center of combustor introduces methane at 80 m/s. Ambient air enters the combustor coaxially at 0.5 m/s. The overall equivalence ratio is approximately 0.76 (28% excess air). The high-speed methane jet initially expands with little interference from the outer wall, and entrains and mixes with the low-speed air. The Reynolds number based on methane jet diameter is approximately $5.7 \times 10^3$. To save a computational cost, only half of the domain is considered since the problem is symmetric. The combustion is modeled using a global one-step reaction mechanism, assuming complete conversion of the fuel to CO\textsubscript{2} and H\textsubscript{2}O. This model is based on the generalized finite-rate chemistry. The reaction equation is

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
This reaction is defined in terms of stoichiometric coefficients, formation enthalpies, and parameters that control the reaction rate. The reaction rate is determined assuming that turbulent mixing is the rate-limiting process with the turbulence-chemistry interaction modeled using the eddy-dissipation model.

3. Mathematical Model

The equation for conservation of mass or continuity equation can be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$  \hspace{1cm} (1).

Conservation of momentum is described by

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g} + \mathbf{F}$$  \hspace{1cm} (2),

where \( \tau \) is the stress tensor, and \( \mathbf{F} \) is an external body force. \( \mathbf{F} \) also contains other model-dependent source terms such as porous-media.

The stress tensor \( \tau \) is given by

$$\tau = \mu \left[ (\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} I \right]$$  \hspace{1cm} (3),
where $\mu$ is the molecular viscosity, $I$ is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

The energy equation is given by

$$\frac{\partial}{\partial t} (\rho e) + \nabla \cdot (\bar{v} (\rho e + p)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_j h_j \bar{J}_j + (\tau \cdot \bar{v}) \right) + Q \quad (4),$$

where $k_{\text{eff}}$ is the effective conductivity ($k + k_t$, where $k_t$ is the turbulent thermal conductivity defined according to the turbulent model used), and $J_j$ is the diffusion flux of species $j$. The first three terms on the right hand side represent energy transfer due to conduction, species diffusion, and viscous dissipation respectively. The last term $Q$ is heat of chemical reactions.

The total energy $e$ is defined as

$$e = h - \frac{p}{\rho} + \frac{V^2}{2} \quad (5),$$

where $h$ is defined for ideal gas which is incompressible as

$$h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (6),$$

where $Y_j$ is the mass fraction of species $j$, and

$$h_j = \int_{T_{\text{ref}}}^T c_{p,j} dT \quad (7),$$

where $T_{\text{ref}}$ is 298.15 K.

For many multicomponent mixing flows, the transport of enthalpy due to species diffusion can have a significant effect on the enthalpy field and should not be neglected. In particular, when the Lewis number for any species is far from unity, neglecting this term can lead to significant errors.

The reaction rates that appear as source terms in the species transport equations are computed from Arrhenius rate expression, from the eddy dissipation model (Magnussen and Hjertager, 1976).
The conservation equation for species transports is given by

\[ \frac{\partial}{\partial t} \left( \rho Y_i \right) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{j}_i + R_i \tag{8}, \]

where \( R_i \) is the net rate of production of species \( i \) due to chemical reaction and

\[ \vec{j}_i = - \left( \rho D_{i,m} + \frac{\mu_t}{Sc_i} \right) \nabla Y_i \tag{9}, \]

where \( Sc_i \) is the turbulent Schmidt number (\( \frac{\mu_t}{\rho D_t} \) where \( \mu_t \) is the turbulent viscosity and \( D_t \) is the turbulent diffusivity). The standard two-equation, \( k-\varepsilon \) turbulence model (Launder and Sharma, 1974) was employed for this study.

4. Results and Discussion

In the first step, grid structure within the computational domain shown in Figure 2 was generated by Gambit which is the processor bundled with FLUENT. The grid resolution is high at the locations where gradients of variables are high. Subsequently simulations were carried out using FLUENT. The results are depicted in terms of contours.

Figure 2: non-uniform grid structure for the problem computations.

Figure 3: temperature contours for the case of gas phase combustion
The computed temperature is shown in Figure 3 for the gas phase combustion of pure air and CH₄. It can be seen in the figure that temperature is very high where the intense reactions take place. The flame propagates towards the downstream while it spread from the symmetrical line of the computational domain. In case of porous combustion, the resulting temperature is illustrated in Figure 4. The temperature is found lower while temperature contour spreads out more widely. This is attributed to the fact that a porous medium has a feature of combusting sub-normal lean mixtures due to intense heat transfer across the solid to preheat the mixture to the temperatures that sustain chemical reactions.

Figure 4: temperature contours for the case of porous combustion.

To get more insight in species transport phenomena, contours of stream functions are plot for the case of gas phase and porous in Figures 5 and 6 respectively. Stream function represents the trajectories of particles in a flow. The porous case gave lower average value of stream function which implies lower flow intensity. This result is attributed to the viscous effect of solid boundaries within the porous structure.
In what follow, the distributions of mass fraction of CH\(_4\) for the two cases are depicted in Figures 7 and 8. CH\(_4\) is consumed due to combustion. In both cases, CH\(_4\) is highly concentrated near the fuel jet entrance while CH\(_4\) is distributed more widely in porous domain than in the gas-phase domain. However, it can be noticed that more CH\(_4\) is consumed for the gas phase combustion. The results are consistent with temperature distribution shown in Figures 3 and 4. More consumptions of CH\(_4\) indicate higher rate of reaction causing greater temperature rise.
Figure 7: CH₄ contours for the case of gas phase combustion.

Figure 8: CH₄ contours for the case of porous combustion.

Figure 9: CO₂ contours for the case of gas phase combustion.

Figure 10: CO₂ contours for the case of porous combustion.
Finally, the distributions of mass fraction of combustion product CO₂ for the two cases are depicted in Figures 9 and 10. It can be observed CO₂ is more concentrated where concentrations of CH₄ are less as CH₄ is being consumed to produce CO₂. Moreover, CO₂ is distributed more widely in porous domain than in the gas-phase domain consistent with CH₄ distribution previously shown in Figure 8.

5. Conclusion

Numerical simulations of methane diffusion combustion in porous burner have been successfully carried out. Several computed field variables considered include temperature, stream function, and species mass fractions. The analysis was done through a comparison with the gas-phase combustion. Porous combustion is found to give lower temperature with more uniform distribution throughout the domain. In addition porous combustion provide greater rate of fuel consumption thereby raising peak temperature. The porous combustion as in a burner is proved wider flame stability limits and can hold an extended range of firing capabilities due to an energy recirculation.

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7. References


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