Computational Analysis on Hydrogen Combustion in Premixed Flame Reactor for Nanoparticle Synthesis

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Introduction

Burners utilizing premixed flames have been used in the industry to synthesize nanoparticles such as carbon black, titania, silica, alumina etc [1,2]. The stabilization of the premixed flame is difficult to be controlled because of the blow-off and flash-back problem. In order to keep the stability of flame, the flame speed must be fast enough for flame propagation speed [3].

It is necessary to understand the physical and chemical phenomena in flame processes for improving the particle properties and the flame reactor designs. Because, in the flame reactor, the nanoparticles are synthesized at the extremely high temperature and in a very short residence time, it is quite difficult to control the properties of particles [4]. The computational fluid dynamics (CFD) have become useful tools to illustrate the profiles of gas temperature, velocity and species concentration, which affect the properties of particles in the flame reactor [5,6].

In this study, the CFD-code FLUENT was used to simulate the gas temperature and velocity inside the hydrogen-air premixed flame reactor. The difference in two geometries of the hydrogen-air premixed flame reactor was compared.

Theory

Fig. 1 shows experimental schematic of (a) the close premixed flame reactor and (b) open premixed flame reactor. The burner (Fig. 1(c)) corresponds to cylinder with 3 coaxial inlets. In Figure 1(a), the premixed reactants (H_2 = 1 % and air = 99 %) with flow rate of 1 l/min was introduced into the reactor (pyrex, height = 35 cm, and diameter = 5.2 cm) at the central inlet of the reactor (Diameter = 2 cm) and H_2 and air with flow rate of 1 l/min were introduced into first and second annuluses, respectively. In Figure 1(b), the premixed reactants (H_2 = 1 % and air = 99 %) with flow rate of 2 l/min was introduced into the reactor (Pyrex, height = 20 cm and diameter = 5.2 cm) at the inlet tube (length = 10 cm and diameter = 2 cm) and H_2 and air with flow rate of 2 l/min were introduced into first and second annuluses, respectively.

The structured grids were created by using GAMBIT software for the computational domain inside the reactor and the governing equations such as mass, momentum and energy balances were solved by FLUENT.

The total mass conservation equation can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \quad (1)$$

where v is the gas velocity and ρ is the gas density. The conservation equations for chemical species, i, such as H_2, O_2, N_2, and H_2O are expressed as follows:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + M_{w,i} R_i, \quad (2)$$

where Y_i is the mass fraction of species, $\overset{\rho}{J}$ is the diffusive flux of specie i, $M_{w,i}$ is the molecular weight of species i and R_i is the Arrhenius molar rate of creation/destruction of species i in the chemical reaction. For the H_2 combustion reaction, R_i can be represented by the following equation,

$$R_i = -1\times10^5 \exp(-0.012/T)C_1C_2 \quad (3)$$

where C_i is the molar concentration of species i (for H_2, $i = 1$, and for O_2, $i = 2$).

The conservation of momentum in the simulation domain is described as

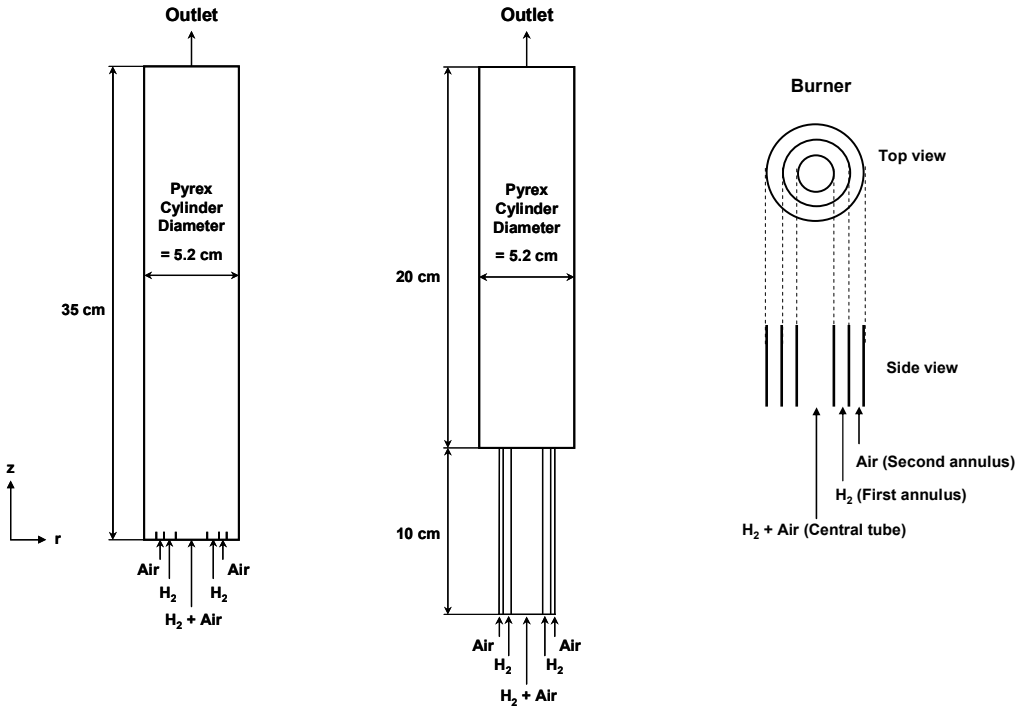
$$\frac{\partial}{\partial t}(\rho\overset{\rho}{v}) + \nabla\cdot(\rho\overset{\rho}{v}\overset{\rho}{v}) = -\nabla p - \nabla\cdot\tau - \nabla\cdot\tau^{(t)} + \rho g + S, \quad (4)$$

where p is the static pressure, τ is the stress tensor, $\tau^{(t)}$ is the turbulent momentum flux tensor, ρg is the gravitational body force and S is the source term.

The energy conservation equation is given as follows:

$$\frac{\partial}{\partial t}(\rho E) + \nabla\cdot(\vec{v}(\rho E + p)) = \nabla\cdot\left[k_{eff}\nabla T - \sum_i h_i\overset{\rho}{J}_i + (\overset{=}{\tau}\cdot\vec{v})\right] + S_h, \quad (5)$$

where E represents the energy, k_{eff} is the effective thermal conductivity, h_i is the enthalpy of species i, and S_h is the source term.



(a) (b) (c)

Fig. 1 Experimental schematic of (a) the close premixed flame reactor, (b) the open premixed flame reactor and (c) burner.

Results and discussion

Fig. 2 shows temperature profiles (K) for various gas flow rates of all gases in the close premixed flame reactor. We assumed the hydrogen combustion reaction to be $2H_2 + O_2 \rightarrow 2H_2O$. The visible flame shape which may be represented by the maximum temperature region is quite flat compared to that of diffusion flame, because the premixed H_2 and air are supplied into the central inlet and combustion reaction takes place immediately in the inlet region. The maximum temperature region appears above the central inlet of the reactor where the premixed combustion reaction of H_2 takes place. We can see the high temperature spots above the side inlets because the non-premixed H_2 combustion takes place in that region. Temperature gradients decrease continuously as the distance is further away from the flame both in axial and radial direction because of heat loss by convection and conduction. With increasing the gas mixture flow rate, high temperature region appears further away from central and side inlets.

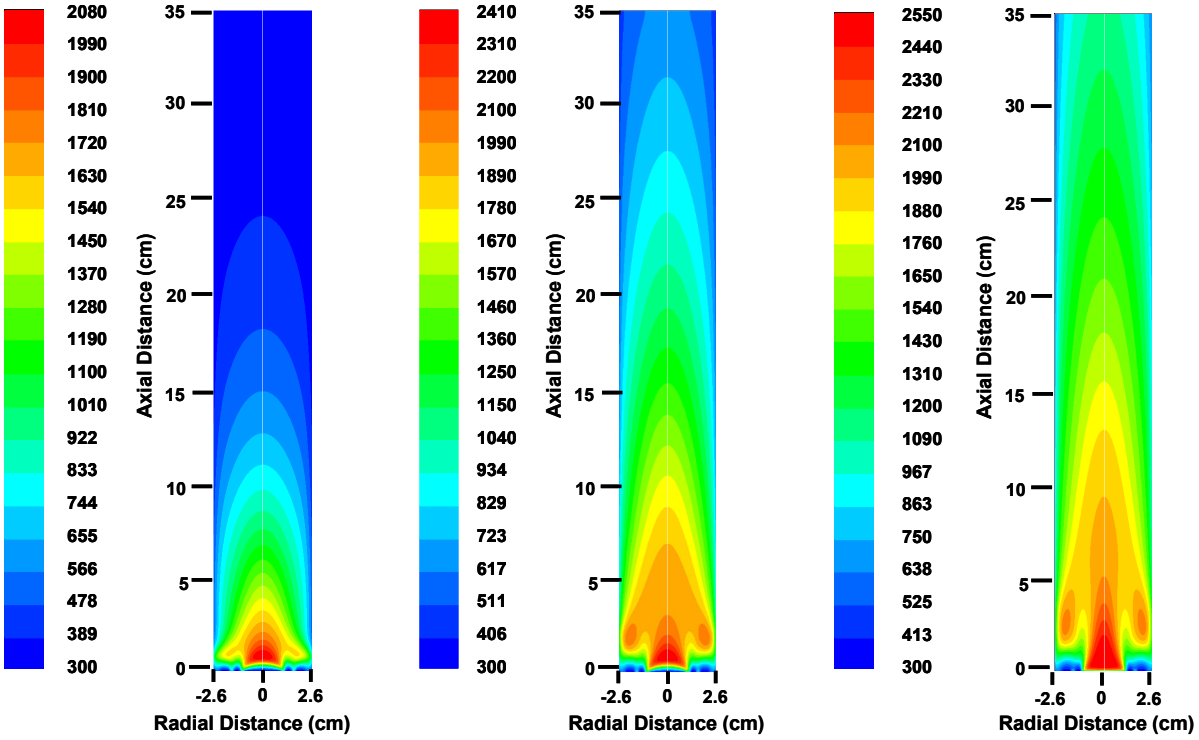


Fig. 2 Temperature profiles (K) for various gas flow rates in all inlets: (a) 1 l/min, (b) 5 l/min and (c) 10 l/min inside the close premixed flame reactor.

Fig. 3 shows temperature profiles (K) for various flow rates of all gases in the open premixed flame reactor. Fig. 3(a) shows that, at low gas flow rate (2 l/min), the highest temperature regions appear at the burner inlet and reactor inlet simultaneously. This phenomenon can be explained by creation of backfire in the burner. In the central tube of the burner, H_2 and air are well mixed and velocity is low, so flame propagation takes place easily in both directions: upward and downward. As the gas flow rate increases (Fig. 3(b,c)), the flame front moves upward along the central tube of burner to the reactor inlet. At gas flow rate of 40 l/min, flame is achieved to the reactor inlet, which is desirable for effective combustion process.

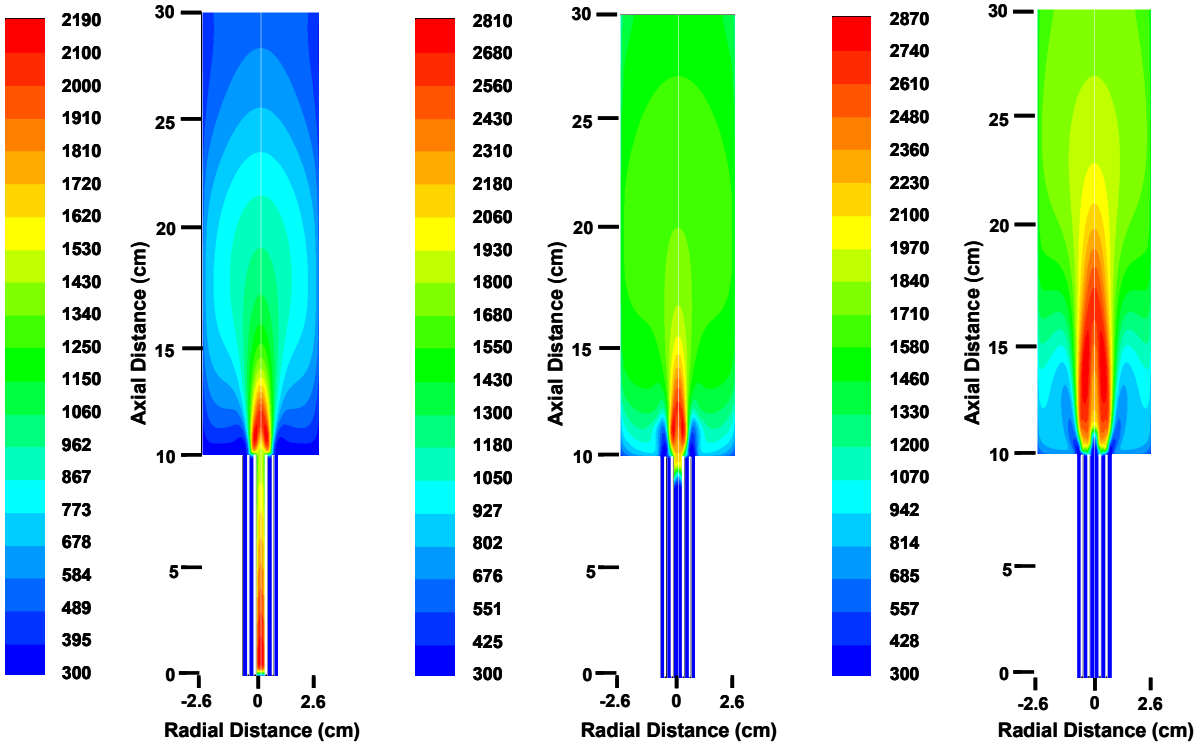


Fig. 3 Temperature profiles (K) for various gas flow rates in all inlets: (a) 2 l/min, (b) 20 l/min and (c) 40 l/min inside the open premixed flame reactor.

Conclusion

In the premixed flame, the flame shape is shorter and flatter than that in the diffusion flame. For the case of close premixed flame reactor, temperature profile is flat at low velocity and the high temperature region becomes higher with increases of gas velocity. In open premixed flame reactor, flame above the burner (without any backfire) could be achieved only at high gas flow rates (more than 40 l/min). The CFD-code FLUENT can be used for simulation of combustion processes inside the premixed flame reactor. It helps to understand the physical and chemical phenomena in flame processes for improving flame reactor designs.

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