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Extinguishment of hydrogen laminar diffusion flames by water vapor in a cup burner apparatus

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ABSTRACT

Transient computations with full hydrogen chemistry were performed to reveal the flame structure and extinguishment process of co-flow, hydrogen diffusion flame suppressed by water vapor. As the concentration of water vapor was increased, the flame detached away from the burner brim and formed an edge flame at the flame base. Water vapor showed larger chemical inhibition effect than nitrogen when extinguishing hydrogen flame, which was attributed to its enhanced third body effect in the reaction $H + O_2 + M = HO_2 + M$. The minimum extinguishing concentration (MEC) of water vapor and nitrogen was predicted by Senecal formula and perfectly stirred reactor (PSR) model respectively. The MECs predicted by PSR model agree with the MECs calculated by Fluent, which shows that 1) the flame extinction is controlled by the flame base, and 2) radiation absorption is negligible. The measured MECs are in a reasonable agreement with the values calculated by Fluent, which demonstrates the accuracy of the CFD model. A simple model was used to investigate the relative importance of extinguishing mechanisms of water vapor. The results show that in a co-flow configuration the thermal cooling and chemical inhibition effect are the main extinguishing mechanisms in suppressing hydrogen diffusion cup burner flame.

1. Introduction

Hydrogen is viewed as a promising clean energy at present, but it is dangerous for its wide explosion range and low-energy ignition. The hazards of hydrogen are a concern in many industries, not only where hydrogen is served as a reactant or product in the chemical industry, but also where hydrogen is an unwanted product in nuclear power plants due to the reaction between zirconium and water (Ingram and et al., 2012; Dobashi, 2014). Many researchers have investigated on the extinguishment/inhibition of hydrogen flame/explosion by some inert gases and ultra-fine water mist (Battersby and et al., 2012; Papas et al., 1994; Ng and Lee, 2008), but few efforts have been paid on the effects of water steam. The lack of interest may be attributed to the fact that the application of water vapor is restricted by its low saturated vapor pressure at room temperature. However, in the chemical or nuclear industry where water steam is used as a primary heat transfer medium, water steam is a potential alternative for ordinary suppressants. The scope of the present study is limited to the interaction of water steam and hydrogen diffusion flames in a cup-burner apparatus at normal atmospheric environment (298 K and 1 atm). This arrangement is based on the following reasons besides of the hydrogen safety. The cup-burner method (Association, 2004) is a widely accepted way to measure gas agents' minimum extinguishing concentration (MEC), which serves as a reference for the design of fire protection systems. Besides, the cup-burner flames are stable and simple enough so that the extinguishing mechanisms can be readily studied.

Some simplified models have been proposed to predict the MECs of gas agents in order to harmonize data used in fire protection standards. Senecal (Senecal, 2005) proposed a phenomenological approach to predict the MECs of inert gases in terms of heat capacity and fuel properties. Zhang et al. (Zhang and Soteriou, 2011) and Liu et al. (Liu and et al., 2008) predicted the MECs of inert and chemical gas agents by using a perfectly-stirred reactor (PSR) model with full chemistry. Linteris et al. (Linteris and et al., 2012) extended the scope of the PSR model to understand the unwanted combustion enhancement by potential halon replacements. Although reasonable agreements are achieved between experiments and calculations, the validity of those models on the

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hydrogen cup-burner flame has not been testified. For laminar hydrogen premixed flame, many experimental and numerical studies have been performed to investigate the extinguishing efficiency and mechanisms of various suppressants. Qiao et al. (Qiao and et al., 2010) simulated the detailed flame structure of premixed hydrogen flame at different suppressant concentrations and found that the third-body reaction $H + O_2 + M = HO_2 + M$ was an important chain-terminating reactions. Seiser et al. (Seiser and Seshadri, 2005) investigated the influences of water on the extinction and ignition of hydrogen/methane premixed flames and found that the addition of water vapor made the hydrogen flames easier to extinguish due to the enhanced chaperon efficiencies of water in reactions $H + O_2 + M = HO_2 + M$, $H + OH = M = H_2O$, and $H + H + M = H_2 + M$. The extinguishing efficiency and mechanisms of various suppressants change with the flame types due to different flame structures and flame speeds. For diffusion flames, Takahashi et al. (Takahashi et al., 2007; Takahashi and Katta, 2009) studied the interaction process of co-flow diffusion flames and fire suppressants in a cup burner. Their results showed that the peak reactivity spot formed at the flame base was crucial for flame stabilization and the extinguishment occurred via a blowoff process rather than the global chemical extinction. Cong et al. simulated the interaction of water steam and methane cup burner flame with one-step chemistry (Cong and Liao, 2008). Their results supported the extinguishing process proposed by Takahashi and further demonstrated that the flame-base oscillation was the key step for flame extinction. It should be noted that hydrogen is free of carbon, and the fact that its combustion product is water indicates water steam's potential capability of curbing specific chemical reactions. Few data have been reported on the MEC of water vapor (MEC_{H2O}) and the relative importance of the extinguishing mechanisms when water steam interacts with hydrogen diffusion flame.

In this study, the hydrogen co-flow diffusion flame was simulated with full chemistry by Fluent and its interaction with water steam was investigated. A PSR model, as well as the Senecal's formula, was used to predict the MECs for hydrogen cup-burner flame. Their results were compared with the Fluent's predicted values and the measured values to confirm the validity of the simplified models and to interpret the influences of different extinguishing mechanisms on MECs. Finally, the relative importance of the extinguishing mechanisms was investigated with an energy balance equation.

2. Experiment and CFD modeling

2.1. Physical model setup

The sketch of the apparatus is shown in Fig. 1(a). The apparatus used here is similar to that in (Cong and Liao, 2008). The cup burner has a cylindrical stainless steel cup and a cylindrical quartz chimney. The bottle of the burner is connected to the TSI atomizer (Model 9306A) through a diffuser. The fuel and air flow rate are measured by a calibrated mass flow meter and vortex flow meter respectively. Their uncertainty is 1% of the indicated flow. For the case of water vapor, the air is preheated before entering the mist chamber. As the air enters the mist chamber, it mixes with ultrafine water mist and passes through an electrically heated fine screen upstream the exit of the cup. The temperature of the fine screen is carefully adjusted to ensure a total evaporation of ultrafine water mist and maintain the temperature of the inlet oxidizer at ≈373 K. The mass flow rate of water vapor equals to that of water mist during the experiments so its value is determined by collecting the water mist at the oxidizer inlet during a given period.

The numerical parameters were set according to the experimental conditions. The stainless steel cup burner had an outer diameter of 31 mm and length of 25 mm while the quartz chimney had an inner diameter of 90 mm and length of 200 mm. The temperature of the quartz wall and burner wall was set at 298 K except the 600 K burner wall within 1 mm away from the top burner brim (Ananth and Mowrey, 2008). No slip boundary condition was applied to the wall. The normal thermal emittance of the hot burner wall and cool wall was 0.24 and 0.22 respectively (Bergman et al., 2011) and the hemisphere integrated radiant emittance was 0.93 for the chimney wall. The initial fuel temperature was 298 K and the inlet velocity of the fuel was fixed at 6.5 cm/s to achieve a laminar flame with a visible flame height of about 75 mm–85 mm (Association, 2004). Three types of oxidizer stream were considered in the simulations, they are: dry air, dry air with nitrogen, dry air with water vapor. The temperature of the inlet oxidizer stream was 298 K and its velocity was fixed at 13.6 cm/s at 1 atm. The mass fraction of the extinguishers in the oxidizer stream was gradually increased to its MEC where the flame sustained combustion.

2.2. The numerical method

The Da number, chemical reaction time t_r and flow time t_f (Quintiere, 2006) were estimated from the following equations:

$$Da = \frac{t_f}{t_r}, \tag{1}$$

$$t_r = \rho C_p T_\infty / [E/RT_\infty] \Delta h_c A e^{-E/(RT_\infty)}, \tag{2}$$

$$t_f = d/v. \tag{3}$$

In these equations, ρ and C_p are the gas density and specific heat capacity near the flame sheet, T_∞ and v is the temperature and velocity of the inlet air, E and A is the activation energy and pre-exponential factor for the hydrogen respectively, Δh_c is the idea heat of combustion and d is the equivalent distance for the air transporting to the flame sheet.

The Da number is nearly 1 at the flame base under the present situations. This means that for the hydrogen cup-burner flame the chemical dynamic effect is at least equivalent to the transport effect. So a detailed reaction mechanism of hydrogen (Ó Conaire and et al., 2004) was incorporated into the laminar finite rate model. The gas phase combustion was solved by the laminar, transient, Navier-Sokes and energy equations with a time step of 0.1 s. The mass diffusion coefficient and thermal diffusion coefficient were calculated by the Chapman-Enskog and kinetic theory respectively. Fluent's DO model was used to account for the radiation loss of the flame. Radiation of the gaseous specie H_2O was incorporated into the model by a polynomial fits and its absorption coefficient was taken from (Peters and Rogg, 1993). The radiation equation was calculated after solving the energy equation for 10 times at each time step.

Fluent solves the conversation equations in finite volume forms. The gradients were computed using Least Squares Cell-Based Gradient method. The diffusion terms in governing equations were discretized by the second–order accurate central-differenced method. The convection terms in momentum equations were discretized using the Fluent's QUICK Scheme and those of the species and energy equations were discretized using a second-order upwind scheme. The coupled pressure–velocity equations were solved using Fluent's PISO method before solving energy and species conservation equations. The residuals for the gas phase energy equation were reduced to 10^{-4}% for convergence while those for other equations were reduced to 10^{-2}% for convergence.