# Numerical Study on the Interaction of Water Mist with a Methane Diffusion Flame

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**Abstract** - A numerical study of the influence of water mist characteristics, such as droplet size and water mist mass flux, on Methane diffusion flame suppression was conducted using CFD method based on Fluent. Water mist was simulated with Eulerian-Lagrangian two phase flow model. The methane diffusion flame was simulated with Finite-Rate/Eddy-Dissipation model. The numerical predicting results show that the predicting temperature in the fire flume is in good agreement with the experimental results which carried out by predecessor. It can also predict the parameters variation such as  $CO_2$ ,  $H_2O$ , CO,  $O_2$  concentration in the process of interaction which could not easily to obtain via experiments. The results indicate that as the mass flux of water mist increased, the temperature of flame decreased significantly, and  $CO_2$  concentration on the flame axis decreased,  $H_2O$  concentration gradually increased, and CO concentration decreased in the bottom but increased around the top of flame which may be caused by the incomplete burning. In addition, water mist can dilute  $O_2$  concentration obviously as its mass flow rate increases.

Keywords: CFD, Water mist, Flame, Mass flux, Two phase flow.

# 1. Introduction

As one of the main substitute for Halon fire extinguishing agents, water mist technology has been developed and received considerable attention all the worldwide. Water possesses many attributes of the ideal fire suppressant. It is non-toxic, non-corrosive, ubiquitous, and has no adverse environmental effects. The mechanisms of fire extinguishment including thermal cooling, oxygen displacement, fuel surface cooling and attenuation of thermal radiation, which have been widely studied in the past years. But about the interaction process between water mist and fire flume, there are still some problem about the suppression mechanisms which have not well solved and understood. There are many researchers who have been investigated the interaction of water sprinkler with fire plume by CFD and achieved many theoretical progresses (John et al., 2006; Gunnar Heskestad, 2002; Soonil Nam, 1996). Recently, many researchers developed the numerical simulation method to study the interaction of water mist or spray with fire plume (Hassan, 1996; Ndubizu et al., 1998; Kuldeep Prasad et al., 1999; Grant et al., 2000; Kuldeep Prasad et al., 2002; Jinsong Hua, 2002; Sung Chan Kim et al., 2003; Yuh-Ming Ferng et al., 2011; Liang Tian-shui et al, 2013).

However, most above studies concerned fire extinguishment efficiency and the water mist system design. There was few work focused on fire suppression mechanisms by water mist via CFD simulation. This paper reports a numerical simulation based on the commercial Fluent software to study the interaction of water mist with a 2D-methane diffusion flame. Comparison of the simulated results with the experiment results (Ndubizu et al.,1998) is also presented.

# 2. Mathematical Model

In this paper, we consider the methane diffusion flame burning in an opening space. It is a typical two phase flow process in the interaction of water mist with fire flame. Gas phase and liquid phase are interacted through the exchange of mass, momentum and energy, and this process was modelled using Eulerian-Lagrangian approach. The standard k- $\epsilon$  turbulence model combining with buoyancy effect was

used. The radiation heat transfer was solved with P1-radiation model. Considering two-step chemical reaction equation of methane, Finite-Rate/Eddy-Dissipation model was used to solve the chemical reaction rate. The interaction of water mist droplets with the fire flume, which includes mass, momentum, energy, components transport, and radiation transfer, was solved through adding the corresponding source term to the gas conservation equations.

#### 2. 1. Gas Phase Model

The methane diffusion flame was generated through free burning in a modified Wolfhard-Parker burner as shown in Fig. 1. Two-step irreversible chemical reaction is assumed:

$$CH_4 + 1.5 O_2 \rightarrow CO + 2H_2 O$$
 (1)

$$\mathrm{CO} + 0.5\mathrm{O}_2 \to \mathrm{CO}_2 \tag{2}$$

The airflow and combustion reaction can be described by the conservation equations of mass, momentum, energy and species along with the sub-models for turbulence and combustion. The governing equations for the gas phase can be expressed in the following general form (Jinsong Hua et al., 2002):

$$\frac{\partial(\rho\phi)}{dt} + \nabla(\rho\vec{U}\phi) = \nabla(\Gamma_{\phi}\nabla\phi) + S_{\phi}$$
(3)

where  $\rho$  (kg/m<sup>3</sup>) is the mixture (fuel, air and hot combustion products) density; u (m/s) is the velocity vector, and t (s) is the time. The symbol  $\phi$  stands for any of the following variables: (1) three velocity components  $u_i$  in the *i*th direction; (2) mass fractions of chemical species  $m_i$ ; (3) enthalpy h; (4) turbulence kinetic energy k; and (5) turbulent dissipation rate  $\varepsilon$ : The definitions of the diffusion coefficient  $\Gamma_{\phi}$  and the source terms  $S_{\phi}$  for the various variables represented by  $\phi$ .



(a) Experimental diagram from Ndubizu et al.(1998) (b) Schematic diagram of the computational domain Fig. 1. Schematic diagram of the water mist interaction with fire plume.

#### 2. 2. Combustion Model

In the current problem of water mist/fire plume interaction, the chemical reaction kinetics in the fire plume is significantly affected by the reaction temperature and reactant concentrations, and may be the dominating factor in the fire extinction mechanism. Therefore, the Arrhenius finite reaction rate model is used in the present study to estimate the combustion rate in fire extinction (Lange et al., 1993):

$$R_{fu} = -A_k T \rho^{\alpha+\beta} m_{fu}^{\alpha} m_{ox}^{\beta} \exp\left(-\frac{E_k}{RT}\right)$$
(4)

where A,  $\alpha$  and  $\beta$  are the model constants, m<sub>fu</sub> and m<sub>ox</sub> are the mass fractions of fuel and oxygen, respectively. *E*(kJ/mol) stands for the activation energy of the chemical reaction,  $\rho$ , *T*, *R* are the gas density (kg/m<sup>3</sup>), temperature (K) and universal gas constant (J/mol • K), respectively.

#### 2. 3. Water Mist Model

The Lagrangian frame treats the water mist as the discrete phase and the fluid phase as the carrier phase using an Eulerian scheme. The fluid phase is treated as a continuous phase by solving the time-averaged N-S equations, while the particle phase is solved by tracking droplets which pass through the calculated flow field.

Fluent predicts the trajectory of a discrete phase droplet by integrating the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written (for the direction in Cartesian coordinates) (Ansys Fluent Theory Guide 14.0, 2011) as,

$$\frac{du_d}{dt} = F_{\rm D}(\vec{u} - \vec{u_d}) + \frac{\vec{g}(\rho_d - \rho)}{\rho_d} + \vec{F}$$
(5)

where  $\overrightarrow{F}$  is an additional acceleration (force/unit particle mass) term,  $F_D(\overrightarrow{u} - \overrightarrow{u_d})$  is the drag force per unit particle mass and  $\overrightarrow{u}$  is the fluid phase velocity,  $\overrightarrow{u_d}$  is the droplet velocity(m/s),  $\mu$  is the molecular viscosity of the fluid (Pa.s),  $\rho$  is the fluid density,  $\rho_d$  is the density of the water droplet (kg/m<sup>3</sup>). The other parameter in the equation was available in (Ansys Fluent Theory Guide 14.0,2011).

Heat and mass exchange between droplets and fire flame is solved by follow equation (Lange et al., 1993):

$$m_d c_d \frac{dT_P}{dt} = A_d h (T_\infty - T_d) + \epsilon_p A_P \sigma \left(\theta_R^4 - T_p^4\right) \left(T_p < T_{vap}\right)$$
(6)

$$m_d c_d \frac{dT_P}{dt} = A_p h(T_{\infty} - T_d) + \frac{d\dot{m}_d}{dt} h_{fg} + \varepsilon_p A_P \sigma \left(\theta_R^4 - T_d^4\right) \left(T_{vap} < T_d < T_{bd}\right)$$
(7)

$$\frac{dD_d}{dt} = \frac{4k_\infty}{\rho_d c_d} \left(1 + 0.23\sqrt{Re_d}\right) \ln\left[1 + \frac{c_{p,\infty}(T_\infty - T_d)}{h_{fg}}\right] \quad (T_{bd} < T_d)$$
(8)

where  $m_d$  is the mass of the droplet (kg),  $c_d$  is the heat capacity of the droplet (J/kg-K),  $A_d$  is the surface area of the droplet (m<sup>2</sup>),  $T_{\infty}$  is the local temperature of the continuous phase (K), h is the convective heat transfer coefficient (w/m<sup>2</sup>-k),  $\varepsilon_d$  is the particle emissivity(dimensionless),  $\sigma$  is the Stefan-Boltzmann constant (5.76×10<sup>-8</sup> w/m<sup>2</sup>-K<sup>4</sup>),  $\theta_R$  is the radiation temperature,  $T_{vap}$  is the vaporization temperature of water(K),  $T_{bd}$  is the boiling temperature of water (K),  $T_d$  is the droplet temperature (K),  $h_{fg}$  is the latent heat of vaporization (J/kg). The other detail information is available in (Ansys Fluent Theory Guide 14.0,2011).

## 3. Physical Model and Numerical Algorithm

A finite-volume method combined with a SIMPLE algorithm was used to solve the whole system. To the droplet phase, the droplets trajectory was obtained through Lagrangian method, and the droplet entered into the computational domain at each time step. Droplet group concept was used to describe water mist moving in the gas phase. The gas phase coupling with the water mist was realized through the source term of energy and mass conservation equation. The objective of this work is to study the variation of the parameters of fire flames when they interact with water mist, where the effects of water mist characteristics on fire suppression was considered. A simplified two-dimensional axisymmetric CFD model was developed to investigate the interaction between fire plume and water mist. The schematic diagram of the computational domain and the experimental diagram (Ndubizu et al., 1998) is shown in Fig. 1. The computational domain was  $40 \times 120$  mm, and non-uniform grid was used. The fuel was burning at the exit of the burner, and the air and water mist have the same flow direction. The cases of this study are shown in Table 1.

Study case	Fuel flow velocity (cm/s)	Air flow velocity (cm/s)	Mass flow rate of water mist (mg/s)	SMD (µm)
Case0(base)	2.8	18.1	0	0
Case1	2.8	18.1	35	30
Case2	2.8	18.1	55	54
Case3	2.8	18.1	15/25/35/45/60	54

Table 1. Para	neters used	in the	simulation.
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# 3. Results and Discussions

Fig. 2 gives the simulated results of the flame temperature above the burner exit at different height of case0. The fuel flow velocity is 2.8 cm/s and the air flow velocity is 18.1 cm/s in the simulation. Due to the low flow velocity, the methane burning was approximately assumed as laminar flame. Fig. 2(a) and Fig. 2(b) show that the simulated results agree well with the experiments. As shown in Fig. 2(c) and (d), with height increase, the predicting width and temperature of the flame are slightly larger than the experimental one, these maybe caused by the approximation of using laminar combustion model.





Fig. 2. Simulated and measured temperature across a methane-air diffusion flame (base case) at different heights without interaction of water mist

Fig. 3 shows the simulated results of flame temperature above the burner exit at different heights of case1. The temperature of flame zone obviously decreases compared with the one without water mist as shown in Fig. 2. The central axis temperatures of the flame 10 mm and 30 mm above the burner exit are a little lower than the experimental results as shown in Fig. 3(a) and Fig. 3(b). It also can be deduced that the flame height inferred from the simulation is higher than the experimental results.



Fig. 3. Simulated and measured temperature of methane-air diffusion flame at different heights with water mist (mass flow rate: 35 mg/s, SMD: 30 µm)

Fig.4 shows the simulation results of flame temperature above the burner exit at different height of case2. Fig.4a shows the temperature of flame axis is very lower in the simulation than experiment at 10mm above the burner exit, and at the same time, the flame width is lager in experiment than the simulation. This may be because the simplified model in simulation makes the water mist obtain certain momentum to across the flame and then enter into the inside of flame, at last absorbs heat due to droplet evaporation. Fig.4b shows that the results of simulation is in good agreement with the experiment at 30mm above the burner exit. Fig.4c shows that the flame temperature is slightly larger in the simulation than the experiment at 45mm above the burner exit. From above, it can be obtained that the flame height is higher in simulation than experiment and the temperature of flame zone decreases compared with case1.



(a) 10 mm above the burner exit
 (b) 30 mm above the burner exit
 (c) 45 mm above the burner exit
 Fig. 4. Simulated and measured temperature of methane-air diffusion flame at different heights with water mist (mass flow rate: 55 mg/s, SMD: 54 µm)

Fig.3 and Fig.4 show the flame temperature of simulation and experiment with water mist and the results show that the simulation can predict the flame temperature on the process of interaction between fire flame and water mist well. Fig.5 shows the variation of flame temperature, H<sub>2</sub>O concentration,CO<sub>2</sub> concentration, CO concentration of the flame axis at different height above the burner exit with different water mist mass flow rate about case3. The temperature of flame axis varies from the maximum value 2020K without water mist to 1650K with water mist under 60mg/s, as the water mist mass flow rate increase, as shown in Fig.5a. Combined with Fig.5b, this indicates that the flame can be suppressed obviously by water mist. As the water mist mass flow rate increase, the H<sub>2</sub>O concentration increases in the flame axis, this is due to water mist entering the internal of the flame with the air entrainment of fire flume, finally the more droplets evaporating leading to the temperature of flame axis decrease and the water vapor concentration increases. From Fig.5c and Fig.5d, we can see that as the water mist mass flow rate increase, the  $CO_2$  concentration decrease, especially at the top zone of the flame. And the CO concentration decreases obviously at the base zone of flame, but increases at the topwhich leads to the decrease of CO<sub>2</sub> concentration. These indicate that the combustion efficiency is affected remarkably by water mist, so concentration distribution of combustion products in the flame will be changed. This can be explained combining with the contours of different species variation in the flame, as shown in Fig.6.





(c) Variation of CO<sub>2</sub> concentration (d) Variation of H<sub>2</sub>O concentration Fig.5. The temperature ,differentspecies concentration of flame axis at different height with different water mist mass flow rate(Case3).

Fig.6a. can further explain the above phenomenon as shown in Fig.5a and Fig.5b. Fig.6b shows that water mist can dilute oxygen concentration in the whole flame zone, especially at the top of flame. From Fig.6c, the CO concentration decreases at the lower part of the flame, but increases at top, and this is due to the incomplete burning at the top of the flame, according to Fig5.d, certainly it cannot be denied that this is the disadvantage sometimes. Because in the study, we use two-step irreversible chemical reaction model, so without water mist, the content of CO concentration is relative large, but it is obviously that when water mist was added, the CO concentration decrease as a whole. So we can find that water mist can suppress the methane diffusion flame effectively from the whole.



(a) Contours of Molar Concentration of  $H_2O(kmol/m^3)$ 



Water mist (25mg/s)





(c) Contours of Molar Concentration of CO(kmol/ m<sup>3</sup>)

Fig. 6. Contours of the H<sub>2</sub>O, O<sub>2</sub>,CO concentration variation with different water mist mass flow rate(Case3)

## 4. Conclusion

A numerical simulation approach based on Fluent has been developed to investigate the interaction between water mist and a methane diffusion flame. From the study, the following conclusions can be drawn:

- (1) The numerical results of flame axis temperature was compared with the experiment by (Ndubizu et al., 1998). And the results of simulation was in good agreement with experiment and indicated that the water mist can lessening the temperature of flame obviously.
- (2) The influence of water mist on the flame structure and different species of flame was investigated through numerical simulation. The results indicate that the temperature and the  $CO_2$ concentration decrease and water vapour H<sub>2</sub>O concentration increases with the water mist mass flow rate increase; the CO concentration decrease at the lower part of flame, but increase at the top, and this is due to the incomplete burning. The water mist also can dilute oxygen concentration and the oxygen concentration was smaller near the flame front with larger water mist mass flow rate. The simulation also indicate that the air entrainment at the top of fire plume is larger than the flame base, so the water mist relatively enter the internal of the top flame easily and the influence on the flame by water mist is relatively obvious. The simulation results prove

that the current approach has the capability to reasonably capture the interactions between the water mist and the fire plume.

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