

# **REVIEW OF MODELING FIRE SUPPRESSION BY WATER SPRAYS BY COMPUTATIONAL FLUID DYNAMICS**

**B.H. Cong and G.X. Liao**

State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei 230026, China

**W.K. Chow**

Department of Building Services Engineering, The Hong Kong Polytechnic University, Hong Kong, China

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## **ABSTRACT**

Water-based fire control systems such as sprinkler are widely used in providing safety. In addition to following the prescriptive codes without understanding the physics behind, more quantitative approaches such as numerical modeling for evaluating the system performance were carried out for new designs. Note that performance-based fire codes might be necessary for some applications. Numerical modeling also contributes to the understanding of the fire extinguishment mechanisms. One of the popular models is Computational Fluid Dynamics (CFD). However, in comparing with applications to simulate fire growth, spread and smoke movement, CFD has not yet been applied extensively to study the fire suppression process or used as a practical design tool. This paper is to review the current developments in using CFD for simulating fire suppression with water sprays. The aim is to provide a broader view on how CFD can be applied for such a study.

Fundamental theories for fire field models will be presented in this paper first. Turbulence, combustion, radiation and chemistry models in application to fire modeling are discussed. More advanced but less applied CFD techniques such as Large Eddy Simulations (LES) will be briefly introduced. Also, water spray models available in the literature are discussed in detail. Two different droplet tracking methods – Eulerian-Lagrangian method and Eulerian-Eulerian method are reviewed. Key issues of fire extinguishment criteria for different scenarios are analyzed. Moreover, CFD modeling of suppressing solid fuels by water sprays, current trends and potential applications of CFD in fire suppression modeling are highlighted. Finally, needs for an extensive study on model development and validation studies are pointed out.

## **1. INTRODUCTION**

Water has been used for controlling fires since the ancient time. That is because water is readily available and inexpensive in most areas. It is nontoxic, and can absorb large amount of heat due to its latent heat of vaporization and high specific heat capacities in both liquid and gas phases.

There are two methods of applying water for firefighting, i.e. jet branch and spray branch. Bulk liquid is applied in the jet branch to cool down the flame and the burning surface using hosereel or fire hydrant systems. Other means such as pouring a basin of water into the fires can also be classified under this method. Large amount of water would be wasted and lead to severe water damages, though jet branch can ‘prewet’ the combustible surface to prevent the ignition. As evaporation can only occur at the liquid surface, it appears that, in theory at least, producing water sprays to extract heat is more desirable for firefighting. In practice, automatic sprinkler system and fixed water spray system are used as fire services installations. Fire suppression with

water sprays is reviewed by Grant et al. [1].

Although water spray systems such as automatic sprinkler have been developed and installed for many years, there are stringent requirements to develop a quantitative approach to evaluate the performance of water spray system under different fire scenarios while implementing performance-based code design. However, carrying out full-scale burning tests is very expensive. Experiments on scale models are restricted by the scaling laws, only good enough for studying smoke movement. On the other hand, Computational Fluid Dynamics (CFD) is now a practical fire engineering tool. There are numerous studies on fire growth, spread and smoke movement reported in the literature. Some of the models [2-5] are validated with experimental data and demonstrated to be successful in predicting smoke movement in rooms, tunnels and warehouses. But this technique is not yet practical for modeling fire suppression.

There had been some progress in applying CFD for modeling fire suppression due to the increase in

computational power and a number of important experiments providing further insight into fire extinction phenomena with water sprays, especially for sprinklers [6-8]. Basic spray dynamics predictions in application to fire studies were studied by Alpert [9], Chow et al. [10,11], and Nam [12,13]. More sophisticated models taking into account the interaction between combustion, radiation and water sprays were also developed [14-17]. The alternative, Eulerian-Eulerian formulation for solving the two-phase flow has been considered by Hoffman and Galea [18-20], Hassan [21] and Prasad et al. [22-24], and tested for several fire suppression scenarios. The current state of CFD modeling for fire suppression is summarized by Novozhilov [25]. However, consistent and satisfactory models of extinguishment are not yet available.

Recently, there are more interests in water mist system, in addition to studying conventional sprinklers. Attention was paid towards gaseous flame mode of suppression. Besides, it is more difficult to study water mist dynamics in comparing with sprinkler sprays. There had been some developments in predicting water mist dynamics and pool fires suppression by Prasad et al. [23]. A limited number of studies using CFD models for full-scale fire suppression research were carried out by Hadjisophocleous et al. [26-28]. But robust algorithms for predicting droplet transport and consistent extinguishment criteria for diffusion flames still remain a problem.

The present review is devoted to CFD modeling of fire suppression with water sprays. The important areas of ignition, fire growth, fire spread and smoke movement will not be discussed. Other firefighting agents such as chemical agents, inert gas agents, and foam agents are also excluded.

This paper is divided into three major sections. Fundamental theories for fire field models will be given in Section 2. Various refinements for turbulence, combustion, radiation and chemistry models are discussed in application to fire modeling.

Section 3 is devoted to a detailed discussion of modeling water sprays. Two different droplet tracking models – Eulerian-Lagrangian method and Eulerian-Eulerian method are discussed in detail. Important issues of fire extinguishment criteria for different scenarios will also be discussed.

Applications of CFD modeling of suppressing solid fuels with water sprays are considered in Section 4. Two distinct methods dealing with burning surface during fire suppression process are concerned. The first method is on simulating gas-droplet flow

only. The solid phase is decoupled from calculations and is represented by a fuel source with spatial and temporary characteristics, which should be obtained from experiments. The second method involves modeling of both gas-droplet and solid phases, thus giving more quantitative information about fire suppression with water sprays.

Some general issues related to fire suppression with water sprays are discussed in the last section. The current state of models development, the gap between theory and practical application and future development are highlighted.

## 2. FUNDAMENTAL THEORY FOR CFD MODELING WITH WATER SPRAYS PART I: FIRE MODELING

In this section, a well-established fire field model based on Favre-averaged Navier-Stokes equations (FANS) with the two-equation closure for turbulence flow is considered. It forms a current ‘standard’ for CFD fire modeling. The basic conservation equations for multi-component reacting flow are given first with the major assumptions, and various submodels are discussed in the subsequent sections. LES-type models are reviewed in the last section.

### 2.1 Conservation Equations

In flows with large variations of density, such as flows with combustion, convenient description is achieved via Favre- (or mass-weighted) averaging [29,30]. In order to close the averaged equations, some models have to be introduced for the Reynolds stress tensor and the turbulence scalar fluxes. The most widely-used models are based on the eddy viscosity hypothesis and the two-equation closure, which is known as  $k-\varepsilon$  closure and involves the two additional partial differential equations for the turbulent kinetic energy  $k$  and the energy dissipation rate  $\varepsilon$ .

The Favre-averaged conservation equations describing the subsonic reacting flow with the model for turbulence may be represented in the following general form,

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla(\rho\mathbf{U}\phi) = \nabla(\Gamma_{\phi}\nabla\phi) + S_{\phi} + S_{p,\phi} \quad (1)$$

The exchange coefficients and the source terms are listed in Table 1. The derivation is not repeated here as these equations are widely accepted for modeling the chemical reacting turbulence flows with low Mach number and relevant discussions are provided elsewhere [31-35].

**Table 1: The flux and source term for the conservation equations**

Dependent variable $\phi$	Diffusion coefficient $\Gamma_\phi$	Source term $S_\phi$	Source term $S_{p,\phi}$
1	0	0	$-\frac{d}{dt}(m_p)$
$u_i$	$\mu_e = \mu + \mu_t$	$-\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu_e \frac{\partial u_j}{\partial x_i} \right) + (\rho - \rho_{ref}) g_i$	$-\frac{d}{dt}(m_p u_{p,i})$
$k$	$\mu_e / \sigma_k$	$P + G - \rho \varepsilon$	0
$\varepsilon$	$\mu_e / \sigma_\varepsilon$	$\frac{\varepsilon}{k} (c_1 [P + c_3 \max(G, 0)] - c_2 \rho \varepsilon)$	0
$Y_F$	$\mu_e / \sigma_Y$	$-C_R \rho \frac{\varepsilon}{k} \min \left( Y_F, \frac{Y_o}{r} \right)$	0
$Y_v$	$\mu_e / \sigma_Y$	0	$-\frac{d}{dt}(m_p)$
$\xi$	$\mu_e / \sigma_\xi$	0	0
$(\xi^n)^2$	$\mu_e / \sigma_\xi$	$c_{g1} \mu_e \left[ \left( \frac{\partial \xi}{\partial x} \right)^2 + \left( \frac{\partial \xi}{\partial y} \right)^2 + \left( \frac{\partial \xi}{\partial z} \right)^2 \right] - c_{g2} \frac{\rho \varepsilon}{k} (\xi^n)^2$	0
$h$	$\mu_e / \sigma_h$	$-Q_R$	$-\frac{d}{dt}(m_p h_p)$

Where:

$$P = \mu_e \left\{ 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 \right] + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)^2 \right\}$$

$$G = g \left( \frac{\mu_e}{\sigma_h} \right) \left( \frac{1}{\rho} \right) \frac{\partial \rho}{\partial z}$$

$$\sigma_k = 0.9, \sigma_\varepsilon = 0.9, \sigma_Y = 0.7, \sigma_h = 0.7, \sigma_\xi = 0.7$$

$$\mu_e = \mu + \mu_t, \mu_t = \rho c_\mu \frac{k^2}{\varepsilon}$$

$$c_\mu = 0.09, c_1 = 1.44, c_2 = 1.92, c_3 = 1.0, C_R = 4.0, c_{g1} = 2.8, c_{g2} = 2.0$$

Eq. (1) is written for a weakly compressible flow, which means that only the fluid density changes as a result of changes in temperature or composition of the mixture, but no pressure. Pressure is, therefore, supposed to be thermodynamically constant and affect the fluid motion only through its spatial derivatives in the momentum equations. Acoustic waves are filtered from the flow. More fundamental issues concerning these equations for fire field modeling are discussed in the literature [36-39].

## 2.2 Turbulence Modeling

The core of the above FANS model is the two equations which provide closure for the turbulence model (equations for the kinetic energy  $k$ , and the energy dissipation rate  $\varepsilon$ ). The basic underlying

assumption for  $k$ - $\varepsilon$  closure is the use of the eddy viscosity model [40,41],

$$-\rho \overline{U'_i U'_j} = -\frac{2}{3} \rho \delta_{ij} k + \mu_t \left( \frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i} \right) \quad (2)$$

$$-\rho \overline{U'_j \phi'} = \frac{\mu_t}{\sigma_\phi} \frac{\partial \overline{\phi}}{\partial x_j} \quad (3)$$

where  $k$  is the turbulence kinetic energy, given as follows,

$$k = \frac{1}{2} \overline{U_i U_i} \quad (4)$$

and  $\sigma_\phi$  is the turbulence Prandtl/Schmidt number for the variable  $\phi$ .

As fire-induced flows are essentially buoyancy-driven, production of turbulence due to buoyancy should be included. This is commonly accomplished by incorporating the additional term according to Rodi [40,41] and Hossain and Rodi [42]. The set of constants for the model, listed in Table 1, are more common and well established, as reviewed by Jones and Whitelaw [38]. However, these parameters are to be adjusted for simulating a particular fire problem [4,43].

Although there are many turbulence models in the CFD literature, models other than the  $k-\epsilon$  model are not so widely used. Algebraic models (one-equation models) which calculated effective viscosity using algebraic functions of mean flow quantities had been used at the early stage of developing fire modeling, but are not so popular now. Reynolds stress models (RSM) have their advantages but they are quite complicated and might cause stability problems in computations due to the stiffness of the equations [44]. The tendency of turbulence models in fire field modeling is concentrated on using the modified versions of  $k-\epsilon$  model and large eddy simulation (LES) technique.

### 2.3 Combustion Modeling

Combustion modeling is related to the heat release, smoke and toxicity gas productions in fires. They are all important aspects from the view of fire safety. In the literature, there are currently three approaches falling essentially into two categories:

- Models based on a conserved scalar approach; and
- Finite reaction rate models.

#### 2.3.1 Fast chemistry conserved scalar approach

Non-premixed, or diffusion flames are focused on under most situations during fire development. A convenient approach dealing with such type of combustion is based on conserved scalars [45]. Conserved scalar allows significant simplifications in the turbulent combustion rate calculations.

For a simple one-step irreversible combustion reaction for hydrocarbon fuel with stoichiometric coefficient  $r$ ,



The conserved scalar can be the mixture fraction, defined as,

$$\xi = \frac{\beta - \beta_o}{\beta_F - \beta_o} \tag{6}$$

where  $\beta$  is also a conserved scalar, given by,

$$\beta = Y_F - \frac{Y_o}{r} \tag{7}$$

Under the additional assumption of equal species diffusivities [29,33] (which is justified in most practically turbulent flows at high Reynolds numbers), the source term for the mixture fraction disappears from the governing equations as shown in Table 1. This equation shows that the mixture fraction behaves as any other conserved scalars, such as inert species.

The conserved scalar approach has achieved much success in combination with a fast chemistry assumption. This assumption is justified in many practically important cases, since many reactions have high rates and can be considered to complete as soon as reactants are mixed. The fast chemistry assumption implies that the reaction time is negligible compared to the fluid mixing time. The instantaneous species concentrations are functions of the conserved scalar. In the simplest case of fast chemistry and one-step irreversible reaction given by Eq. (5), the following relationships hold,

For  $\beta \leq 0$ ,  $\xi \leq \xi_s$  :

$$\begin{cases} Y_F = 0 \\ Y_o = rY_B(\xi_s - \xi) \\ Y_{pr} = (r + 1)Y_B\xi(1 - \xi_s) \end{cases} \tag{8}$$

and

For  $\beta \geq 0$ ,  $\xi \geq \xi_s$  :

$$\begin{cases} Y_F = Y_B(\xi - \xi_s) \\ Y_o = 0 \\ Y_{pr} = (r + 1)Y_B\xi_s(1 - \xi) \end{cases} \tag{9}$$

where

$$Y_B = Y_F / (1 - \xi_s) \tag{10}$$

The stoichiometric value of the mixture fraction  $\xi_s$  corresponds to  $\beta = 0$  and is given by,

$$\xi_s = \frac{Y_o}{rY_F + Y_o} \tag{11}$$

It is assumed here that oxidant and fuel cannot exist together.

The problem of chemistry-turbulence interaction is drastically simplified in the fast chemistry conserved scalar approach. Mean Favre-averaged concentrations can be obtained by integrating the appropriate Favre Probability Density Function (PDF) for the conserved scalar over the mixture fraction space to include the effect of turbulence fluctuations as follows,

$$\bar{Y}_i(\mathbf{x}) = \int_0^1 Y_i(\xi) \bar{P}(\xi; \mathbf{x}) d\xi \quad (12)$$

Generally, transport equation for the PDF may be solved to account for its dependence on flame location, turbulence and other parameters [46]. A simple and currently widely used method in fire modeling approach is to assume a general form of the PDF with variable parameters that relate to the first and second moments of the conserved scalar. For this purpose, an additional equation is solved, as shown in Table 1, for the variance of the mixture fraction,

$$\overline{(\xi')^2} = \overline{(\xi - \bar{\xi})^2} \quad (13)$$

The most widely used forms of PDFs are the Beta function and the clipped-Gaussian distribution. The PDF transport equation is described in detail in the literature [33,46].

### 2.3.2 Eddy break-up approach

The fast chemistry approach to combustion is generally widely used for fire modeling [47-49]. However, the eddy break-up approach has become a more popular choice recently [25]. In the eddy break-up (EBU) model, an extension of the conserved scalar approach is achieved by taking into consideration a second variable, which concentration is affected by the chemical kinetics. The eddy break-up model was originated from the works of Spalding [50,51] and subsequently developed by Magnussen and Hjertager [52].

If the chemical reaction rate is controlled by the rate of molecular mixing of reactions, which in turn is related to the rate of dissipation of turbulent eddies, then the mean rate of fuel consumption can be written as follows [50],

$$R_f \sim \rho \left( \frac{\varepsilon}{k} \right) \bar{Y}_F'^2 \quad (14)$$

Such an expression requires calculation of the instantaneous fuel concentration. Magnussen and Hjertager [52] related this instantaneous quantity to

the mean flow quantities which resulted in a closed model. In diffusion flames, fuel and oxygen occur in separate eddies. Because fuel and oxidant appear as fluctuating intermittent quantities, there should be a relationship between the instantaneous and the mean species concentrations. Consequently, the rate of fuel consumption can be expressed as,

$$R_f \sim \bar{Y}_F \left( \frac{\varepsilon}{k} \right) \quad (15)$$

However, in the fuel rich regions of the flame, oxidant will show strong intermittency. Thus, the combustion rate is limited by the dissipation of the oxygen eddies according to the expression similar to Eq. (15),

$$R_f \sim \frac{\bar{Y}_o}{r} \left( \frac{\varepsilon}{k} \right) \quad (16)$$

The final expression or the reaction rate may be written in the form,

$$R_f = -C_R \rho \frac{\varepsilon}{k} \min \left( \bar{Y}_F, \frac{\bar{Y}_o}{r} \right) \quad (17)$$

A further controlling term might be added to limit the rate of reaction at low temperatures. This is necessary in the extinguishment modeling studies,

$$R_f = -C_R \rho \frac{\varepsilon}{k} \min \left( \bar{Y}_F, \frac{\bar{Y}_o}{r}, \bar{Y}_F \bar{Y}_o A_p \exp \left( \frac{-E}{RT} \right) \right) \quad (18)$$

Obviously, fuel mass fraction serves as a second variable along with mixture fraction in the EBU model. Therefore, the transport equation for the fuel mass fraction, as shown in Table 1, is solved under this approach, instead of that for the mixture fraction variance.

The distribution of oxidant and products are given by

$$Y_o = 1 - Y_F - \frac{\xi - Y_F}{\xi_s} \quad (19)$$

$$Y_{pr} = 1 - Y_F - Y_o$$

Although the EBU model is popularly used in fire applications, detailed kinetics of combustion cannot be included.

### 2.3.3 Finite reaction rate approach

The fast chemistry assumption is not always applicable. The production of many important species in turbulence flames is controlled by the

intermediate chemistry. Therefore, finite rate kinetic effects should be modeled. A straightforward way to incorporate finite rate chemistry is based on the laminar flamelet models. As no attempt has yet been made to apply this technique to fire suppression modeling, the finite reaction rate will not be reviewed in this paper. Further information is provided in the literature [53,54].

## 2.4 Thermal Radiation

Radiation exchange plays a very important role in fires, might even be a dominant mode of heat transfer [55]. Besides, the attenuation of thermal radiation by water droplets is an important extinguishing mechanism for water mist [56,57]. Therefore, the effects of radiation and the interaction of droplets and radiation should be included in studying fire suppression with CFD.

### 2.4.1 Basic radiant transport equation

The fundamental quantity of radiation transport is the spectral intensity  $I_\lambda$ . This is defined as the radiant energy (per unit time per unit wavelength interval) passing per unit surface area normal to the direction into a unit solid angle  $\Omega = (\theta, \varphi)$  centered around  $\Omega$ .

For an absorbing/emitting and scattering medium, the radiant transport equation (RTE) at position  $\mathbf{x}$  in the direction  $\mathbf{s}$  is written as [58],

$$\frac{dI_\lambda(\mathbf{x}, \mathbf{s})}{ds} = -\alpha_\lambda(\mathbf{x})I_\lambda(\mathbf{x}, \mathbf{s}) - \sigma_\lambda^s(\mathbf{x})I_\lambda(\mathbf{x}, \mathbf{s}) + \alpha_\lambda(\mathbf{x})I_{\lambda,b}(\mathbf{x}) + \frac{\sigma_\lambda^s(\mathbf{x})}{4\pi} \int_0^{4\pi} I_\lambda(\mathbf{x}, \mathbf{s}')\Phi(\mathbf{s}, \mathbf{s}')d\Omega' \quad (20)$$

where  $\mathbf{x}$  is position vector,  $\mathbf{s}$  is direction vector,  $\mathbf{s}'$  is scattering direction vector,  $s$  is the path length,  $I_{\lambda,b}(\mathbf{x})$  is the Planck function describing the spectral intensity of blackbody radiation,  $\Omega'$  is the solid angle,  $\Phi(\mathbf{s}, \mathbf{s}')$  is the scattering phase function that gives the scattered intensity from direction  $\mathbf{s}$  to  $\mathbf{s}'$ .  $\alpha_\lambda(\mathbf{x})$  is the absorption coefficient, and  $\sigma_\lambda^s(\mathbf{x})$  is the scattering coefficient. Both of them are functions of wavelength, chemical compositions of the medium, temperature and pressure. Summing up the two coefficients will give the extinction coefficient:

$$K_\lambda(\mathbf{x}) = \sigma_\lambda^s(\mathbf{x}) + \alpha_\lambda(\mathbf{x}) \quad (21)$$

Eq. (20) is a first-order integral-differential equation. It is very difficult to solve in its general

form since each direction and each wavelength must be considered separately. The second problem is on accurate determination of absorption and scattering coefficients. This requires detailed knowledge of the atomic and molecular properties of the medium. Mathematical approaches are, therefore, developed introducing certain simplifications.

### 2.4.2 Computational methods for radiant transport equation

There are four approaches used to model the radiation heat transfer in the literature for fire field models. The simplest calculation is based on the observation that a roughly fixed proportion of the total heat release will be radiated by the diffusion flames, which depends on the type of the fuel. This global radiation model, the so-called "constant- $\chi$ " approach, was developed by Markstein [59] and exploited in a number of studies. The constant fraction of the radiation emitted  $\chi$  is obtained from experiments. Then, the total enthalpy definition can be modified using the parameter  $\chi$  to give reasonable maximum flame temperatures, which take into account the radiant heat loss. Such approach might be too simple and not suitable for studying the effect of radiation on water sprays. More accurate models should involve solution of simplified forms of Eq. (20).

One of the simplifications employed is a gray gas assumption, which implies that absorption and emission coefficients are independent of the wavelength of radiation. This greatly simplifies the calculations. The equation of radiant heat transport is deduced, if scattering is neglected, to

$$\frac{dI(\mathbf{x}, \mathbf{s})}{ds} = (\alpha_g(\mathbf{x}) + \alpha_s(\mathbf{x}))I(\mathbf{x}, \mathbf{s}) + \frac{\sigma}{\pi}(\alpha_g(\mathbf{x}) + \alpha_s(\mathbf{x}))I^4 \quad (22)$$

for total intensity:

$$I(\Omega) = \int_0^\infty I_\lambda(\Omega)d\lambda \quad (23)$$

The overall absorption coefficient is split into gas and the soot absorption coefficients.

Three major computational methods employed to solve this simplified radiant transport equation are the flux method, discrete transfer method and discrete ordinates method. The first two have been widely used in fire modeling, with advantages and disadvantages discussed by Novozhilov [25]. In this paper, only the discrete ordinates method is discussed.

In the discrete ordinates method, the radiant transport equation is solved for a finite number of discrete solid angles, each associated with a vector direction fixed in the globe Cartesian system ( $x, y, z$ ). The fineness of the angular discretization is controlled by the user, analogous to choosing the number of rays for the discrete transfer method. Unlike the discrete transfer method, it is not necessary to perform ray tracing. Instead, Eq. (22) is transformed into an equation for radiation intensity in the spatial coordinates ( $x, y, z$ ). The solution method is identical to that used for fluid flow and energy equations.

The radiant transport equation is written in the direction  $\mathbf{s}$  in terms of the spatial coordinates  $x_i$ ,

$$\begin{aligned} \frac{d(I_\lambda(\mathbf{x}, \mathbf{s})s_i)}{dx_i} = & -\alpha_\lambda(\mathbf{x})I_\lambda(\mathbf{x}, \mathbf{s}) - \sigma_\lambda^s(\mathbf{x})I_\lambda(\mathbf{x}, \mathbf{s}) \\ & + \alpha_\lambda(\mathbf{x})I_{\lambda,b}(\mathbf{x}) + \frac{\sigma_\lambda^s(\mathbf{x})}{4\pi} \int_0^{4\pi} I_\lambda(\mathbf{x}, \mathbf{s}')\Phi(\mathbf{s}, \mathbf{s}')d\Omega' \end{aligned} \quad (24)$$

where  $s_i$  are the components of  $\mathbf{s}$ . Details of the computational procedure are reported in the literature [60].

### 2.4.3 Radiation attenuation by droplets

Thermal radiation attenuation of water droplets is a combination of scattering and absorption [57]. Accurate prediction of the radiation field and the droplet energy balance would require a good understanding of radiation effects on droplets.

Scattering and absorption effects of water droplets will give a radiation transfer equation,

$$\begin{aligned} \frac{dI_\lambda(\mathbf{x}, \mathbf{s})}{ds} = & -(\alpha_{\lambda,g}(\mathbf{x}) + \alpha_{\lambda,d}(\mathbf{x}))I_\lambda(\mathbf{x}, \mathbf{s}) - (\sigma_{\lambda,g}^s(\mathbf{x}) + \sigma_{\lambda,d}^s(\mathbf{x}))I_\lambda(\mathbf{x}, \mathbf{s}) \\ & + \alpha_{\lambda,g}(\mathbf{x})I_{\lambda,b}(\mathbf{x}) + \alpha_{\lambda,d}(\mathbf{x})I_{b,d}(\mathbf{x}) \\ & + \frac{\sigma_{\lambda,g}^s(\mathbf{x})}{4\pi} \int_0^{4\pi} I_\lambda(\mathbf{x}, \mathbf{s}')\Phi(\mathbf{s}, \mathbf{s}')d\Omega' \\ & + \frac{\sigma_{\lambda,d}^s(\mathbf{x})}{4\pi} \int_0^{4\pi} I_\lambda(\mathbf{x}, \mathbf{s}')\Phi(\mathbf{s}, \mathbf{s}')d\Omega' \end{aligned} \quad (25)$$

where  $\alpha_{\lambda,d}$  is the droplet absorption coefficient,  $\sigma_{\lambda,d}^s$  is the droplet scattering coefficient and  $I_{b,d}$  is the emission term of the droplets.  $\Phi(\mathbf{s}, \mathbf{s}')$  is the scattering phase function that gives the scattered intensity from direction  $\mathbf{s}$  to  $\mathbf{s}'$ . The local absorption and scattering coefficients are calculated from the local droplet number density

$N(\mathbf{x})$  and mean diameter  $d_m(\mathbf{x})$  as:

$$\alpha_{\lambda,d}(\mathbf{x}) = N(\mathbf{x}) \int_0^\infty f(r, d_m(\mathbf{x})) C_a(r, \lambda) dr \quad (26)$$

$$\sigma_{\lambda,d}^s(\mathbf{x}) = N(\mathbf{x}) \int_0^\infty f(r, d_m(\mathbf{x})) C_s(r, \lambda) dr \quad (27)$$

where  $r$  is the droplet radius,  $\alpha_{\lambda,d}$  and  $\sigma_{\lambda,d}^s$  are absorption and scattering cross-sections respectively given by Mie theory. The droplet number density function  $f(r, d_m)$  is assumed to have the same form as the droplet size distribution, but a different meaning.

The in-scattering integral on the right-hand side of Eq. (25) is approximated by dividing the total solid angle  $4\pi$  into a ‘‘forward angle’’  $\delta\Omega^f$  and an ‘‘ambient angle’’  $\delta\Omega^* = 4\pi - \delta\Omega^f$ . Within  $\delta\Omega^f$ , the intensity  $I_\lambda(\mathbf{x}, \mathbf{s})$  is approximated by,

$$U^*(\mathbf{x}, \lambda) = \frac{U(\mathbf{x}, \lambda) - \delta\Omega^f I_\lambda(\mathbf{x}, \mathbf{s})}{\delta\Omega^*} \quad (28)$$

where  $U(\mathbf{x})$  is the total integrated intensity.

The in-scattering integral can be written as:

$$\begin{aligned} \frac{\sigma_{\lambda,d}^s(\mathbf{x})}{4\pi} &= \int_0^{4\pi} I_\lambda(\mathbf{x}, \mathbf{s}')\Phi(\mathbf{s}, \mathbf{s}')d\Omega' \\ &= \sigma_{\lambda,d}^s(\mathbf{x}) [\chi_f I_\lambda(\mathbf{x}, \mathbf{s}) + (1 - \chi_f) U^*(\mathbf{x})] \end{aligned} \quad (29)$$

where  $\chi_f$  is a fraction of the total intensity originally within the solid angle  $\delta\Omega^f$ , that is scattered into the same angle  $\delta\Omega^f$ . Details of the computation of the above simplified radiation transport equation are given in the literature [61].

## 2.5 Large Eddy Simulation

Large eddy simulation (LES) modeling is a relatively new tool in studying engineering fluid dynamics problems. Attempts to use large eddy simulation for fire modeling have been made in the last years, but further work is still required. Recent studies have demonstrated very encouraging results, and this technique is likely to be a focus of fire models in the next decade.

### 2.5.1 Basic concepts of large eddy simulation

As turbulence flow contains a wide range of length and time scales, they all cannot be resolved in most practically important cases. LES makes use of the fact that the large-scale eddies are generally more energetic than the small ones, thus providing much

more effective transport of conserved properties. It is feasible to resolve large-scale motion more accurately than small-scale motion. In LES, large-scale motion is solved exactly, and approximated modeling is required only for small-scale motion. Small eddies contain only a small portion of the total turbulence kinetic energy. Therefore, the computed flows are usually less sensitive to the approximations involved in the small-scale turbulence modeling. Furthermore, small eddies tend to be more universal in character, thus giving more reliable models.

LES approach was started from the pioneering works of Lilly [62] and Deardoff [63]. Since then, there has been a considerable success in applying this technique for studying many flow problems in a wide variety of engineering and geophysics applications.

As described in above, large-scale eddies are computed directly. Therefore, the equation governing the large-scale behavior of flow variables must be derived first. This is done by filtering the Navier-Stokes equations to remove the scales of motion irresolvable on the computational mesh. A homogeneous filter is defined by the convolution integral,

$$\bar{\phi}(x,t) = \int_A G(\mathbf{X} - \mathbf{X}'; \Delta) \phi(\mathbf{X}', t) d\mathbf{X}' \quad (30)$$

where the filter kernel,  $G$ , is a localized function. Different forms of filters may be applied, such as Gaussian, box filter, or a cutoff, which eliminates all Fourier coefficients belonging to wave numbers above a cutoff. In any case, some length smaller than  $\Delta$  is associated with each filter. Eddies with size larger than  $\Delta$  are solved, eddies of the size below  $\Delta$  is modeled. An obvious requirement is that the grid cell size  $h$  satisfies the condition of  $h < \Delta$ .

The filtered non-dimensional Navier-Stokes equations for compressible flow with chemical reactions are written as follows [64],

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} U_j}{\partial X_j} = 0$$

$$\frac{\partial \bar{\rho} U_i}{\partial t} + \frac{\partial \bar{\rho} U_i U_j}{\partial X_j} = -\frac{\partial \bar{p}}{\partial X_i} + \frac{1}{\text{Re}} \frac{\partial \bar{\tau}_{ij}}{\partial X_j}$$

$$\frac{\partial \bar{\rho} e}{\partial t} + \frac{\partial \bar{\rho} e U_j}{\partial X_j} = -p \frac{\partial \bar{U}_j}{\partial X_j} + \frac{1}{\text{Re}} \tau_{jk} \frac{\partial U_j}{\partial X_k}$$

$$+ \frac{1}{M^2 \text{RePr}} \frac{\partial}{\partial X_j} \left( \frac{\mu}{\gamma - 1} \frac{\partial T}{\partial X_j} \right) + \frac{1}{\gamma M^2} \sum_{i=1}^N h_i \bar{\dot{\omega}}_i^* \quad (31)$$

$$\bar{p} = \frac{\bar{\rho} T}{\gamma M^2}$$

where the internal energy per unit mass  $e$  is:

$$e = \frac{T}{\gamma M^2 (\gamma - 1)} \quad (32)$$

and the viscous stress tensor  $\tau_{ij}$  is:

$$\tau_{ij} = \mu \left( \frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} - \frac{2}{3} \delta_{ij} \frac{\partial U_k}{\partial X_k} \right) \quad (33)$$

Since

$$\overline{U_i U_j} \neq \bar{U}_i \bar{U}_j \quad (34)$$

Modeling is required for the quantity known as subgrid scale (SGS) Reynolds stress  $\tau_{ij}^s$ ,

$$\tau_{ij}^s = -\rho (\overline{U_i U_j} - \bar{U}_i \bar{U}_j) \quad (35)$$

It should be noted that the name ‘stress’ reflects the way in which it is treated, rather than the physical nature of this quantity. The models, which are used to approximate SGS Reynolds stress, are called subgrid scale SGS models.

A reasonably successful SGS model was proposed by Smagorinsky [65], relating SGS Reynolds stress to the strain-rate tensor of the resolved scales through a SGS eddy viscosity  $\mu_s$ ,

$$\tau_{ij}^s = \mu_s \left( \frac{\partial \bar{U}_i}{\partial X_j} + \frac{\partial \bar{U}_j}{\partial X_i} \right) + \frac{1}{3} \tau_{kk}^s \delta_{ij} = 2\mu_s \bar{S}_{ij} + \frac{1}{3} \tau_{kk}^s \delta_{ij} \quad (36)$$

Dimensional analysis gives:

$$\mu_s = C_s^2 \rho \Delta^2 |\bar{S}| \quad (37)$$

where  $C_s$  is the model parameter and  $\Delta$  is the filter length scale.

In general,  $C_s$  may be a function of Reynolds number and other non-dimensional parameters. Different values of  $C_s$  are used in different flows. For this reason, the best results are obtained with the advanced Smagorinsky-type of SGS models [66].

There are other terms in the general set of Eq. (31) which require modeling. The pressure-dilatation term and the dissipation function are the examples, as discussed in the literature [64].

### **2.5.2 Application of LES in fire modeling – FDS (Fire Dynamics Simulator)**

LES is a relatively new technique and its application to fire studies has been limited. The studies carried out so far employed further simplified assumptions in order to predict large-scale fire-induced flows. Most of the simulation works were two-dimensional [67-69]. As turbulence is essentially a three-dimensional phenomenon, this significantly reduced their legitimacy but the most general features of the flow would be predicted.

The most consistent effort to apply LES to fire research has been reported by Baum and co-workers [70-74]. A software Fire Dynamics Simulator (FDS) has been developed and updated frequently, which is available free and can be downloaded from the website <http://fire.nist.gov/fds/>.

An approximate form of the Navier-Stokes equations appropriated for low speed, thermal driven flow with emphasis on smoke spreading and heat transfer in fires is used in FDS. The approximation involves filtering acoustic waves while allowing for large variation in temperature and density. This gives a set of elliptic equations, consistent with low speed, thermal convective processes. The computation can either be treated by Direct Numerical Simulation with the dissipative terms computed directly; or as Large Eddy Simulation. The basic equations for FDS are available in the literature [61].

FDS has been applied in modeling fire dynamics in compartments and outdoors. It has also been used to study the interaction between water sprinkler, smoke, heat vent and draft curtain [75-77]. The intention was not to simulate in depth the two-phase interaction of air and droplets from a single sprinkler, nor to predict the suppression of the fire itself, but to study the effect of dozens of sprinklers on a fire-driven flow field in enclosures. Results agreed quantitatively well with the tests on heptane spray burner in terms of both predicting the sprinkler to be within about 15% of the experiments for the first ring, and 25% for the second. The gas temperatures near the ceiling were predicted to be within 15%. Another study on modeling water mist fire suppression system applied to shipboard compartment was reported by Sean et al. [78]. Results showed that FDS predicted the compartment temperature well in some cases, but only fairly good for the average

temperature. Although predicted bulkhead temperature agreed with the experiments, fire extinguishment cannot be predicted. Modifications to the combustion model are necessary.

## **3. FUNDAMENTAL THEORY FOR CFD MODELING WITH WATER SPRAYS PART II: WATER SPRAYS MODELING**

The second phase – water droplet phase in fire suppression modeling with water sprays will be discussed in this section. A brief introduction to quantitative characterization of water sprays will be given in Section 3.1. Two different droplet tracking models – Eulerian-Lagrangian method and Eulerian-Eulerian method are discussed in Sections 3.2 and 3.3 in detail. Important issues concerned with fire extinguishment criteria in different fire scenarios are discussed in Section 3.4.

### **3.1 Quantitative Characterization of Water Sprays**

Quantitative measurement of spray droplet size is required to study the heat transfer of fight-fighting sprays. Such a parameter is also fundamental in defining other attributes of the spray. In this section, spray characterization will be reviewed. Details of the available methods for modeling droplet size distributions will be given. This is important for modeling fire suppression with water sprays.

#### **3.1.1 Spray characterization**

There are two fundamental physical quantities associated with a given droplet: its diameter and its velocity. Both of them are used as initial conditions for modeling.

Water droplets in a given spray can be subdivided into classes. Each class consists of droplets of diameters within a certain range of a given diameter  $D$ . By counting the number of droplets in each class, it is possible to construct a histogram of the frequency of occurrence of a given class. Fitting the histogram by a continuous curve is the probability density function of the droplet size, or the droplet size distribution function. The process above describes the number distribution; but it is also possible to construct area and volume distributions. The velocity distribution function can be constructed in a similar manner.

In general, the breakup of bulk fluid results in a spray where the sizes of droplets are distributed between some non-zero minimum diameter and a

finite maximum diameter. For convenience, most droplet size distributions assume that the droplet diameters range from zero to infinity. In this case, for the droplet size distribution to be physically valid, it is necessary to satisfy the following conditions:

$$\lim_{D \rightarrow 0} \int_0^D f(D) dD = 0, \quad \lim_{D \rightarrow \infty} \int_0^D f(D) dD = 0 \quad (38)$$

and

$$f(D) \geq 0, \quad \int_0^{\infty} f(D) dD = 1 \quad (39)$$

For simplification, it is often desirable to characterize a particular droplet size distribution in terms of a single number, or a representative droplet diameter. The polydisperse distribution is thus replaced with a monodisperse one, where the diameter of each droplet is equal to the appropriate representative droplet diameter. The representative size of the droplets has been standardized by Mugele and Evans [79]. Various mean diameters can be calculated from the following equation:

$$D_{p,q} = \left[ \frac{\int_0^{\infty} D^p f(D) dD}{\int_0^{\infty} D^q f(D) dD} \right]^{1/(p-q)} \quad (40)$$

**Table 3: Mathematical droplet size distributions**

Droplet size distribution	$f(D)$
Normal droplet size distribution	$\frac{1}{\sqrt{2\pi}s_n} \exp\left[-\frac{1}{2s_n^2}(D-\bar{D})^2\right]$ where: $s_n$ is standard deviation; $\bar{D}$ is mean droplet size.
Log-normal droplet size distribution	$\frac{1}{\sqrt{2\pi}Ds_g} \exp\left[-\frac{1}{2s_g^2}(\ln D - \ln \bar{D}_{ng})^2\right]$ where: $s_g$ is geometric standard deviation; $\bar{D}_{ng}$ is geometric mean droplet size.
Nukiyama-Tanasawa droplet size distribution	$aD^p \exp(-bD)^q$ where: $a, b, p, q$ are independent constants.
Rosin-Rammler droplet size distribution	$1-Q = \exp(-(D/X)^q)$ where: $Q$ is the fraction of the total volume contained in droplet diameter less than $D$ ; $X$ and $q$ are constants, for most sprays the value of $q$ lies between 1.5 and 4.

The following diameters are commonly used in water sprays: the arithmetic mean diameter  $D_{10}$ ; the volume mean diameter  $D_{30}$ ; and the Sauter mean diameter  $D_{32}$ . Specific applications of these mean droplet diameters are summarized in Table 2 [80].

**Table 2: Mean droplet diameters for specific applications**

Mean diameter	Symbol	Application
Arithmetic	$D_{10}$	Comparisons
Volume	$D_{30}$	Hydrology: volume control
Sauter	$D_{32}$	Mass transfer and reaction rates

**3.1.2 Mathematical droplet size distribution functions**

In the absence of any fundamental theory to develop droplet size distributions, several functions were proposed based on either probability or empirical expressions. This gives mathematical representation of the measured droplet size distributions. Normal, log-normal, Nukiyama-Tanasawa, Rosin-Rammler, and upper-limited distributions, shown in Table 3, are used [81]. As the basic mechanisms involved in atomization are not yet clearly understood, there is no single distribution function which can represent all droplet size data. It is necessary to test several distribution functions to give the best fitting curve with experimental data.

### 3.2 Eulerian-Lagrangian Method

The Eulerian-Lagrangian method for simulating two-phase flow has been investigated in detail [82-85]. The gas phase is regarded as a continuum while the liquid droplet phase is treated as individual particles traced by the Lagrangian approach. Key elements of this technique in modeling of water sprays will be discussed in this section.

#### 3.2.1 Equations of motion for droplets

The equation of a single spherical droplet motion in turbulent flow field forms the base of Lagrangian modeling for sprays. In a general form, this equation may be taken as [32]:

$$\begin{aligned} \frac{\pi}{6} d_p^3 \rho_p \frac{d\mathbf{U}_p}{dt} = & \frac{\pi}{8} d_p^2 \rho C_D |\mathbf{U} - \mathbf{U}_p| (\mathbf{U} - \mathbf{U}_p) + \frac{\pi}{6} d_p^3 \rho \frac{d\mathbf{U}}{dt} \\ & + \frac{\pi}{12} d_p^3 \rho C_1 \frac{d}{dt} (\mathbf{U} - \mathbf{U}_p) \\ & + \frac{3}{2} d_p^2 (\pi \rho \mu)^{1/2} C_B \int_0^t \frac{(d/d\xi)(\mathbf{U} - \mathbf{U}_p)}{(t-\xi)^{1/2}} d\xi + \mathbf{F}_e \end{aligned} \quad (41)$$

The terms on the right-hand side represent, respectively:

- drag;
- force due to static pressure gradient;
- virtual-mass term;
- basset force to account for effects of deviation of the flow from a steady flow pattern around the sphere; and
- external body-force, e.g. gravity.

Detailed considerations of the relative importance of each term are provided by Faeth [83]. The effect of lift force and Magnus effect are ignored here. And for water spray application, the pressure gradient term may be neglected, as it is generally small for spray processes.

For dilute water spray, such as sprinkler, the simplified equation of droplet motion for water sprays may be taken as [86]:

$$\frac{d\mathbf{U}_p}{dt} = \left( \frac{3\rho C_D}{4d_p \rho_p} \right) (\mathbf{U} - \mathbf{U}_p) |\mathbf{U} - \mathbf{U}_p| + \mathbf{g} \quad (42)$$

where  $\rho$  is the density of the gas phase,  $\rho_p$  is the density of the particle phase,  $\mathbf{U}_p$  and  $\mathbf{U}$  are the velocity of the two phases, and  $C_d$  is the drag coefficient.

There have been numerous studies on the correlations for the drag coefficient. The most

widely used is the one by Putnam [87].

$$C_D = \begin{cases} \frac{24}{\text{Re}_p} \left( 1 + \frac{\text{Re}_p^{2/3}}{6} \right) & \text{for } \text{Re}_p < 1000 \\ 0.44 & \text{for } \text{Re}_p > 1000 \end{cases} \quad (43)$$

where the particle Reynolds number  $\text{Re}_p$  is based on the droplet diameter:

$$\text{Re} = d_p |\mathbf{U} - \mathbf{U}_p| / \mu \quad (44)$$

#### 3.2.2 Turbulent dispersion of droplets

Turbulent dispersion of the droplets can be modeled by the stochastic discrete particle approach. In addition, this approach can be combined to model a set of clouds about a mean trajectory that includes the effects of turbulence fluctuations in the gas phase velocities [82].

In the stochastic discrete particle model, the interaction of a particle with a succession of discrete stylize fluid phase turbulent eddies is simulated. Each eddy is characterized by:

- A Gaussian distributed random velocity fluctuation,  $u'$ ,  $v'$  and  $w'$
- A time scale,  $\tau_e$

The values of  $u'$ ,  $v'$  and  $w'$  that prevail during the lifetime of turbulent eddy are sampled by a Gaussian probability distribution,

$$u' = \zeta \sqrt{u'^2} \quad (45)$$

where  $\zeta$  is a normally distributed random number, and the remainder of the right-hand side is the local rms value of the velocity fluctuations. Assuming isotropy, these values can be obtained as:

$$\sqrt{u'^2} = \sqrt{v'^2} = \sqrt{w'^2} = \sqrt{2k/3} \quad (46)$$

for the  $k$ - $\varepsilon$  model. The selection of characteristic lifetime of the eddy had been discussed in the literature [82].

#### 3.2.3 Heat and mass transfer equations

The heat transfer equation must be considered for droplet in order to describe the history of droplet temperature and evaporation rate in fire environment. Assuming uniform temperature inside the droplets, this equation takes the form [88]:

$$\frac{d(m_p c_p T_p)}{dt} = \dot{q}_c + L \frac{dm_p}{dt} \quad (47)$$

where  $\dot{q}_c$  is the convective heat transfer around the droplet given by:

$$\dot{q}_c = h_c A (T_g - T_d) \quad (48)$$

and the rate of the droplet evaporation is given by:

$$\frac{dm_p}{dt} = -Sh\pi d_p \frac{k_g}{c_{p,g}} \ln(1 + B_m) \quad (49)$$

where the heat transfer number  $B_m$  is taken as:

$$B_m = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}} \quad (50)$$

It is assumed that the partial pressure of vapor at the droplet surface corresponds to the saturation conditions at a given temperature.

The Ranz-Marshall correlations are commonly used to calculate the Nusselt and Sherwood numbers, which govern the heat and mass transfer processes. These are given as functions of Reynolds, Prandtl and Schmidt numbers [89,90]:

$$\begin{aligned} Nu &= 2.0 + 0.6 Re_p^{1/2} Pr^{1/3} \\ Sh &= 2.0 + 0.6 Re_p^{1/2} Sc^{1/3} \end{aligned} \quad (51)$$

The heat transfer equation also includes the boiling rate of a water droplet by the following equation [17]:

$$\begin{aligned} \frac{dd_p}{dt} &= \frac{4k_g}{\rho_d C_{p,g} d_d} \left(1 + 0.23\sqrt{Re_d}\right) \ln\left(1 + \frac{C_{p,g}(T_g - T_d)}{L}\right) \\ (T_d &\geq T_{b,p}, d_d > 0) \end{aligned} \quad (52)$$

$$\dot{m}_b = \frac{1}{2} \rho_d \pi d_d^2 \frac{dd_d}{dt}$$

### 3.2.4 Integration of the trajectory equation

The trajectory equation and any auxiliary equations describing heat or mass transfer are solved by stepwise integration over discrete time steps. Integration of the equation of motion for the droplet in time yields the droplet velocity at each point along the trajectory itself,

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}_p \quad (53)$$

During the integration, the fluid phase velocity  $\mathbf{U}$  is taken as the velocity at the particle position.

### 3.2.5 Coupling between the discrete and continuous phases

In order to get a coupled solution between gas and droplet phase, the Particle-Source-In-Cell (PSI) model [25] is used. Particles are treated [91] as sources of mass, momentum and energy in the continuum phase. The equations for each phase are solved with the particle source terms updated until a converged solution between the phases is achieved. Full details of the technique are provided in the literature [85].

### 3.2.6 Fire suppression predictions with Eulerian-Lagrangian method

For Eulerian-Lagrangian method, a number of studies have been made on CFD modeling of sprinkler sprays interaction with the hot fire plume. Basic characteristics of fire plume/spray interaction were established in a simplified form in early works of Alpert [9]. The water flux which penetrates through the plume, as well as the cooling effect of the spray were calculated. The results were found to be well correlated by the ratio of the initial vertical component of the spray thrust to the maximum upward thrust of the fire plume. Similar integral spray parameters such as the drag to plume buoyancy ratio and the total amount of heat loss had been used by Chow and Fong [10].

Detailed studies on predicting the Actual Delivered Density (ADD) were reported by Nam [12,13]. The actual delivered densities for two early suppression fast response sprinklers (ESFR) were predicted at four different water flow rates and different fire burning rates. The agreement between predictions and measurements was reasonably good. As expected, predictions over the larger area were more accurate than those over the smaller one. These computational tests clearly demonstrated that ADD can be predicted with sufficient accuracy in real fire situations. Spray interaction with the fire plume was also predicted reasonably well. Momentum of the spray as a function of a distance from the deflector, axial velocity of the plume and axial temperature distribution in the plume were generally within few percent of the measured data. The results suggested that the current sprinkler models were capable of quantitative predictions of water spray/fire interaction, and might be developed further to simulate fire suppression.

There are several physical and chemical suppression mechanisms which act simultaneously during spray operation. Major mechanisms have been identified and discussed as follows [92]:

- Heat extraction;
- Oxygen displacement; and
- Blocking of radiant heat.

Heat extraction has an effect on both the pyrolysis reaction which produces flammable volatiles, and the diffusion flame reaction in the gas phase. Oxygen displacement affects mainly gas phase combustion reaction due to mixture dilution with water vapor. Radiation attenuation due to the presence of water droplets and vapor reduces thermal feedback to the fuel, and therefore, decreases the burning rates and prevents ignition of the unburned fuel.

Currently, there is no computational model which takes into account all the major mechanisms described above. Fire suppression modeling is mainly restricted to the effects of heat extraction in the literature. Models for extinguishment of PMMA plate and simple wood cribs were reported by Novozhilov et al. [14,15]. All three phases (gas, water spray and burning solid material) are fully coupled. The predictions were validated against large-scale fire extinguishment experiments carried out in a wind tunnel.

Along with the direct extinguishment modeling, there are other problems concerning sprays/fire interaction. One of the problems is the destabilization and ‘knock-down’ of smoke layer by a spray which brings smoke to lower levels of compartment and is, therefore, a concern from the safety point of view. Sprinkler-hot layer interactions were studied by Chow and Cheung [11]. Air flow patterns, temperature and smoke concentrations were compared at different locations. The results showed better agreement for locations far from the fire source than for locations close to it. Neither combustion nor droplet evaporation was included in the model, which probably caused large deviations from experimental data at some locations.

### 3.3 Eulerian-Eulerian Method

An alternative technique for two-phase flow is the Eulerian-Eulerian formulation, where both phases are treated as interspersed continua occupying the same space, and their share of space is measured by their volume fraction. The two phases interact with each other via friction, heat and mass transfer. This approach has been less exploited in fire studies than Eulerian-Lagrangian formulation. Details of the general Eulerian-Eulerian formulation can be found in the literature [93,94]. Specific application of this approach to fire/water spray interaction modeling has been presented in the literature [18-24].

Generally, a set of nonlinear partial differential equations is to be solved for the following variables:

- Gas phase and particulate phase velocity;
- Pressure;
- Enthalpies for gas and particulate phases;
- Water vapor concentration within the gas phase;
- Gas and particulate volume fractions;
- “Shadow” volume fraction, i.e. the volume fraction which would be occupied by droplets in the absence of evaporation. The shadow volume fraction technique allows the evaluation of the diminishing droplet size during evaporation;
- Turbulence model parameters (e.g. turbulence kinetic energy and its dissipation rate for the  $k-\varepsilon$  model).

The precise formulation of the differential equations describing the model will not be presented here, as those review works are available in some textbooks [e.g. 93]. However, the general vector form of the equation will be presented. Turbulence in the liquid phase is always neglected.

#### 3.3.1 Basic differential equations

- Continuity equations

$$\frac{\partial}{\partial t}(r_i \rho_i) + \nabla \cdot (r_i \rho_i \mathbf{U}_i) = r_i S_i \quad (54)$$

where  $i$  refers to the phase of interest (1 for gas, 2 for liquid). The volume fractions  $r_1$  and  $r_2$  need to satisfy the “space sharing” condition,

$$r_1 + r_2 = 1 \quad (55)$$

The source/sink term (source for the gaseous phase and sink for liquid phase)  $S_i$  is the rate of evaporation.

- Conservation equation for the general variable  $\phi$

$$\frac{\partial}{\partial t}(r_i \rho_i \phi_i) + \nabla \cdot (r_i \rho_i \mathbf{U}_i \phi_i - r_i \Gamma_{\phi_i} \nabla \phi_i) = r_i S_{\phi_i} \quad (56)$$

where  $\phi_i$  stands for the general dependent variables (velocities, enthalpy, etc.). Equations for these various quantities differ primarily in the way in which the terms  $\Gamma_{\phi_i}$  and  $S_{\phi_i}$  are connected with other variables. They are derived from Eq. (56) simply by replacing  $\phi_i$ ,  $\Gamma_{\phi_i}$  and  $S_{\phi_i}$  with appropriate expressions. The precise

form of the diffusion coefficients  $\Gamma_{\phi_i}$  and source term  $S_{\phi_i}$  can be found in the literature [19].

### 3.3.2 Auxiliary equations

Necessary correlations describing the interactions between the phases must be introduced to close the problem. These relations deal with the inter-phase heat and mass transfer, and friction between the gas and liquid phases. Gas and droplets are assumed to be dispersed over the solution domain and the droplets are spherical [19,21]. The last assumption is not essential but simplifies the nature of the empirical input.

- Inter-phase friction coefficient

The two phases, gas and liquid, “slip” with respect to each other resulting in the inter-phase-friction force, which is of the form,

$$F = \frac{1}{2} C_d \rho_g A_p |\mathbf{U}_{slip}|^2 \quad (57)$$

where  $\rho_g$  is the density of the gas phase,  $C_d$  is the drag coefficient,  $\mathbf{U}_{slip}$  is the slip velocity given by:

$$|\mathbf{U}_{slip}| = \left( (u_1 - u_2)^2 + (v_1 - v_2)^2 + (w_1 - w_2)^2 \right)^{1/2} \quad (58)$$

and  $A_p$  is the total projected droplet area of the liquid phase present in the cell given by:

$$A_p = (1.5V / d_p) r_2 \quad (59)$$

where  $d_p$  is the droplet diameter, and  $V$  is the volume of the cell.

The drag coefficient  $C_d$  is evaluated as follows for  $Re < 10^5$  [19].

$$C_d = \max \left[ 0.42, \frac{24}{Re} (1 + 0.15 Re^{0.687}) + \frac{0.42}{1.0 + (4.25 \times 10^4) Re^{-1.16}} \right] \quad (60)$$

where **Re** is the particle Reynolds number given by,

$$Re = d_p |\mathbf{U}_{slip}| / \mu \quad (61)$$

- Inter-phase mass transfer coefficient

As this problem deals with evaporating water droplets, the loss of the droplets needs to be calculated. Several mass transfer models are suggested. The inter-phase mass transfer is given by:

$$\dot{m} = bA(Y_{v,s} - Y_{v,g}) \quad (62)$$

where  $Y_{v,s}$  and  $Y_{v,g}$  are the concentrations of water vapor at the interface and in the gas, respectively. The mass transfer coefficient  $d_p$  is taken as a function of the Sherwood number:

$$b = (ShD) / d_p \quad (63)$$

The Ranz and Marshall correlation for evaporating water droplets may be used to calculate the Sherwood number [89,90].

To close the problem, water vapor concentrations at the interface and in the gas may be calculated according to the following relationships:

$$\begin{aligned} Y_{v,s} &= (M_w p_{sat}) / RT_s \\ Y_{v,g} &= (M_w H_m p_{sat}) / RT_g \end{aligned} \quad (64)$$

- Inter-phase heat transfer coefficient

The concept of an interface between the two phases, with the temperature  $T_s$ , is introduced to describe the heat exchange between the gas and the droplets. Using this temperature, the rates of heat transfer from the gas to the interface, and from the interface to the particle interior are evaluated as follows:

$$\begin{aligned} q_{g \rightarrow s} &= h_g A (T_s - T_g) \\ q_{s \rightarrow l} &= h_l A (T_s - T_l) \end{aligned} \quad (65)$$

where  $h_g$  and  $h_l$  are the heat transfer coefficients between the gas and the interface, and between the interface and the liquid, respectively;  $A$  is the interface area per computational cell.

These heat transfer coefficients are evaluated using the following relationships:

$$h_g = Nuk_g / d_p \quad h_l = 3k_l / (d_p / 2) \quad (66)$$

The interface or particle surface temperature is obtained from the energy balance over a control volume enclosing the interface.

The above relationships are based on convection heat transfer only. When there is mass transfer, latent heat of evaporation should be accounted for in the heat balance equation. The heat transferred from the gas to the surface of the droplet is given by [19]:

$$q_{g \rightarrow s} = \dot{m} [C_{p,g} (T_s - T_g) + L] \quad (67)$$

### 3.3.3 Droplet calculations

- Droplet size calculation

The method proposed by Spalding to be used for finite difference calculations, known as the “shadow” volume-fraction method, was designed to compute an average particle size as follows [95,96]. The conservation for the second phase can be written as:

$$r_2 \sum g_{2o} = \sum r_{2i} g_{2i} - \dot{m} \quad (68)$$

where  $r_2$  is the volume fraction of phase 2 within a control cell,  $r_{2i}$  is the volume fraction in the neighboring cells from which fluid enters the control cell,  $g_2$  is the mass flux of phase 2, and  $\dot{m}$  is the rate of mass transfer from phase 2 to phase 1. The subscripts  $i$  and  $o$  denote inflow and outflow from a control cell respectively.

Further calculation is required to obtain the shadow volume fraction  $r_s$ , defined as the fraction of the volume where the second phase would have occupied in the absence of mass transfer,

$$r_s \sum g_{s2o} = \sum r_{si} g_{2i} \quad (69)$$

The average diameter of the droplets within each control cell can be evaluated using the relation

$$d_d = d_m \left( \frac{r_2}{r_s} \right)^{1/3} \quad (70)$$

where  $d_m$  is the initial average diameter of the droplets injected into the system.

- Surface temperature calculation

The surface temperature of the droplet is evaluated using the equation [96]

$$T_s = \frac{a_1 T_1 + a_2 T_2 + \dot{m} C T_2}{a_1 + a_2 + \dot{m} C} \quad (71)$$

where  $a_1$  is the gas-to-surface-of-droplet heat transfer coefficient and  $a_2$  is the surface-to-the-interior-of-droplet heat transfer coefficient.

### 3.3.4 Fire suppression predictions with Eulerian-Eulerian method

Application of this type of modeling has been limited, compared to the Eulerian-Lagrangian formulation. Two fire suppression scenarios in real compartments were studied by Hoffmann et al. [18-20]. Volumetric heat source with time

varying heat release rate was used to simulate the fire. The comparison between the predicted and measured temperatures indicated rather good agreement at locations near the sprinkler source, but not in the far field. The evolution of a life-threatening zone, in which temperature exceeds 50 °C below 1.5 m level from the floor, was also followed. The development and spread of this hot layer could be monitored during unsteady simulations. However, radiative heat transfer and combustion had not been included in the models.

Fine water spray for the extinction of fires in computer cabinets was reported by Hassan [21]. Mixture fraction combustion model and discrete transfer radiation model were involved to simulate the fire. The water spray discharge mode following the method of Chow and Fong [10] was simulated as a cone-shaped pattern, which was assumed to be unaffected by the gas flow, and no droplet trajectories calculations were involved. Only the heat coupling between the water spray and the fire was considered. The results showed good agreement with the experimental data without the water spray application. However, the model with fine water spray was not validated.

CFD modeling of fire suppression with water mist was done by Prasad et al. [22-24]. Three configurations of methane-air diffusion flame, methanol liquid fires, and large compartment fire suppression with water mist were studied. A complete set of unsteady, compressible Navier-Stokes equations was solved along with an Eulerian sectional water mist model. Parametric studies are performed to determine the effect of mist density, injection velocity and droplet diameter on fire suppression effectiveness with water mist, which is considered contributing to optimize the system design.

## 3.4 Fire Extinguishment Criteria

Many fire extinguishment criteria have been used in the literature. For example, Williams [97] discussed fire suppression from the viewpoint of a critical Damkohler number (defined as the ratio of the residence time of the reactions in the flame to the chemical reaction time) below which extinction occurs abruptly. Coralett and Williams [98] introduced a length scale of coherent flaming with successful suppression being considered as a reduction of the coherent length below a critical value. Rasbash [92,99] discussed extinguishment using water in terms of fire point (which is defined as the temperature below which diffusion burning can no longer be possible). Critical pyrolysis rates (which is defined as the minimum pyrolysis rate to sustain the steady combustion) were used by Yang [100] to analyze extinguishment processes of solid fuel fires using water sprays. Recently,

Mawhinney [101] summarized three parameters introduced to describe the fire extinguishment with water mist: Limiting Adiabatic Flame Temperature (LAFT), Limiting Oxygen Concentration (LOC) and Lower Flammability Limit (LFL). However, there is not much information on proper extinguishment criterion for a specific fire scenario in the literature.

#### 4. CFD MODELING OF FIRE SUPPRESSION OF SOLID COMBUSTIBLES WITH WATER SPRAYS

In Section 2 and Section 3, the basic theory for fire suppression with water sprays, mainly focusing on spray dynamics in fire environment, has been discussed in detail. However, in order to model fire suppression of solid combustibles, which is considered to be three-phase reactive flow, the models concerned with solid fuel combustion and interaction with spray droplets are necessary to exploit. When the water droplets reach the burning surface, simple transfer corrections become more difficult to apply. The reason for this is that water is not only cooling the surface and surrounding gas, but it is also changing the pyrolysis rate of the fuel. In the literature, two methods have been adopted. The first method deals with the simulation of gas-droplet flow only, so that the solid phase is decoupled from calculations and is represented by a fuel source with spatial and temporary characteristics. The second group of studies involves modeling of both gas-liquid phase and solid phase, and allows discussing important issues regarding fire suppression modeling.

##### 4.1 The Empirical Model

Most of the work in this area were performed at Factory Mutual and has been adopted in FDS software. The model is based on the work done by Yu et al. [102]. Dozens of rack storage commodity fires of different geometries and water spray application rates were considered, and the suppression rates were characterized in terms of a few global parameters. From the analysis, an expression was obtained for the total heat release rate from a storage fire after sprinkler activation:

$$\dot{Q} = \dot{Q}_0 e^{-k(t-t_0)} \quad (72)$$

where  $\dot{Q}_0$  is the total heat release rate at the time of application  $t_0$ , and  $k$  is a fuel-dependent constant.

For the FMRC Standard Plastic commodity,  $k$  is

given as:

$$k = a_1 \dot{m}_w'' + a_2 \quad (73)$$

where  $\dot{m}_w''$  is the flow rate of water impinging on the box tops, divided by the area of exposed surface.  $a_1$  and  $a_2$  are constants related to the fuel type.

This analysis is based on the globe water flow rate and burning rates, which is not suitable for CFD modeling. However, the exponential nature of suppression by water was observed both locally and globally, thus it was assumed that the local burning rate of fuel can be expressed [103] as:

$$\dot{m}_f''(t) = \dot{m}_{f,0}''(t) e^{-\int k(t) dt} \quad (74)$$

where  $\dot{m}_{f,0}''$  is the burning rate when no water is applied and  $k(t)$  is a linear function of the local water mass per unit area  $m_w''$  expressed by:

$$k(t) = a m_w''(t) \quad (75)$$

Note that  $a$  is an empirical constant.

##### 4.2 The PDE Model

If the surface of the fuel is planar, it is possible to characterize the decrease in the pyrolysis rate as a function of the decrease in the total heat feedback to the surface. The work on this subject was mainly reported by Novozhilov et al. [14,15]. An unsteady prediction method for suppression with wood and a steady formulation associated mapping method for suppression with thermal thick materials such as PMMA have been established. Details are not to be presented here. However, some limitations need to be noted here:

- The simplified wood pyrolysis model adopted in the study was very sensitive to a number of kinetic parameters, might only be valid for suppression of earlier fires.
- One dimensional heat transfer equation may be suitable for planar fires. While, in general, three-dimensional heat transfer should be taken into account.
- The instant volatiles escape assumption may not be proper during the process of water droplets interaction with solid surface. A porous pyrolysis model may be introduced.
- The mode of water droplets interaction with solid surface was not included in any studies, which may be involved in future work.

## 5. CONCLUSIONS

The progress made in the last decades in fire science, computational methods and computer performance made it possible to extend the use of CFD technique from pure academic use to practical engineering. The increasing trend towards performance-based regulation and accessibility of computer power and software tools also support wider engineering implementation of CFD methods. However, for fire suppression with water sprays, attempts were made on the interaction of spray and fire plume dynamics. Few studies were on extinguishment modeling. Most of the work were not yet validated by experiments. Therefore, there is no confidence to evaluate the fire extinguishing system performance using CFD modeling.

As for models, problems involving turbulence, combustion and its related issues have long been studied by the combustion community. Advanced techniques such as LES and CMC Conditional Moment Closure (CMC) methods may be adopted in fire modeling. However, the motivation for most research by combustion community has been the improvement of efficiency in industrial processes and power plants, where combustion is under control. Fire, by contrast, is essentially uncontrolled combustion. So any attempt to overly constrain the processes under investigation will be proved counterproductive. They will provide information for combustion science, but not for fire science.

Relative crude water suppression submodels have been incorporated into various CFD-based models over the past decades. Thus far, the models can be used for qualitative analysis of sprinkler and water mist suppression systems. Further studies in this area should be continued to give more detailed physical features. Note that the least understood submodel would affect the accuracy of the model, challenges to modelers are to develop more consistent and satisfactory extinguishment submodels.

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## NOMENCLATURE

$a_i$  Numerical coefficients  
 $A_p$  Pre-exponential factor; total projected area

of the liquid phase within control volume  
 $b$  Mass transfer coefficient  
 $B$  Burner width  
 $B_m$  Spalding's mass transfer number  
 $c_p$  Specific heat  
 $C_B$  Basset force coefficient  
 $C_D$  Drag coefficient  
 $C_l$  Virtual mass drag coefficient  
 $C_R$  Eddy-Breakup constant  
 $D$  Diffusivity  
 $d_p$  Droplet diameter  
 $e$  Specific internal energy  
 $E$  Activation energy  
 $f$  Linear branching coefficient  
 $F_e$  External body force  
 $G$  Filter kernel  
 $\mathbf{g}$  Gravity acceleration vector  
 $h$  Enthalpy  
 $h_c$  Convective heat transfer coefficient  
 $H$  Height of compartment/tunnel  
 $I$  Radiation intensity  
 $I_\lambda$  Spectral intensity of radiation  
 $I_{\lambda b}$  Planck function  
 $K$  Turbulence kinetic energy; thermal conductivity  
 $k_b$  Boltzmann constant  
 $K_\lambda$  Extinction coefficient  
 $L$  Latent heat of phase change  
 $L_e$  Dissipation length scale  
 $M$  Mach number  
 $m'$  Burning rate  
 $\dot{m}$  Mass transfer rate  
 $m_{vol}$  Mass flux of volatiles  
 $M_w$  Molecular weight of water  
 $n$  Particulate concentration of active particles involved in soot formation  
 $n_0$  Spontaneous origination rate of active particles  
 $N$  Particulate concentration of soot  
 $N_0$  Avogadro's number  
 $Nu$  Nusselt number  
 $p$  Pressure  
 $P$  Probability Density Function  
 $Pr$  Prandtl number  
 $q$  Heat flux  
 $\dot{q}$  Volumetric heat release rate  
 $Q_p$  Heat of pyrolysis  
 $Q_R$  Heat source due to radiation  
 $\mathbf{r}$  Oxidant stoichiometric requirement for fuel; volume fraction  
 $r_s$  Oxidant stoichiometric requirement for soot  
 $R$  Universal gas constant  
 $Re$  Reynolds number  
 $Re_p$  Particle Reynolds number  
 $s$  Distance along the radiation ray  
 $Sc$  Schmidt number  
 $S_{ij}$  Strain-rate tensor  
 $S_\phi$  Source term for variable  $\phi$   
 $S_{p\phi}$  Source term for variable  $\phi$  due to particles

$t$	Time
$t_e$	Turbulence eddy lifetime
$t_p$	Particle transit time through the eddy
$T$	Temperature
$\mathbf{U}$	Velocity vector
$vol$	Cell volume
$\mathbf{X}$	Cartesian coordinate
$Y$	Mass fraction

**Greek symbols**

$\alpha$	Absorption coefficient
$\beta$	Soot particle coagulation rate
$\gamma$	Ratio of specific heats
$\Gamma_\phi$	Exchange coefficient for variable $\phi$
$\varepsilon$	Turbulence kinetic energy dissipation rate
$\delta_{ij}$	Kronecker's symbol
$\Delta$	Filter width
$\eta$	Kolmogorov scale of turbulence
$\kappa$	Linear termination coefficient
$\mu$	Dynamic viscosity
$\mu_s$	Subgrid scale eddy viscosity
$\sigma$	Stefan-Boltzmann constant
$\sigma^s$	Scattering coefficient
$\sigma_\phi$	Prandtl/Schmidt number for variable $\phi$
$\nu$	Kinematic viscosity
$\rho$	Density
$\phi$	Any variable
$\dot{\omega}_i^*$	Chemical reaction rate
$\chi$	Scalar dissipation rate
$\xi$	Mixture fraction
$\tau$	Viscous stress tensor
$\tau^s$	Subgrid scale Reynolds stress tensor
$\theta, \varphi$	Spherical coordinates
$\Omega$	Solid angle
$\Lambda$	Computational domain

**Subscripts**

$ab$	Absorption
$e$	Effective
$em$	Emission
$F$	Fuel
$g$	Gas
$i$	ith species; ith vector component
$l$	Liquid
$lam$	Laminar
$O$	Oxygen
$p$	Particle
$pr$	Production
$rad$	Radiation
$ref$	Reference
$s$	Stoichiometric; soot; solid; surface
$sat$	Saturation
$scat\_in$	Scattering in
$scat\_out$	Scattering out
$slip$	Slip velocity between phases
$t$	Turbulence

$\lambda$	Wavelength
$\infty$	Free stream

**Superscripts**

'	Fluctuation with respect to Reynolds mean
"	Fluctuation with respect to Favre mean
$e$	Equilibrium

**Overbar symbols**

—	Reynolds averaging; filtered quantity
$\sim$	Favre averaging

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