Chapter 17
CFD Modeling of Tunnel Fires

Abstract Computational fluid dynamics (CFD) modeling has been widely used for performance-based tunnel fire safety design in engineering applications. A CFD tool divides a computation domain into a large number of small cells, and solves a set of differential equations with sub-models using different solution algorithms. The CFD users need to not only efficiently use CFD tools, but also to understand the embedded mechanisms. The basics of CFD modeling are introduced including controlling equations, different turbulence models, and numerical methods. Sub-models important for tunnel fires are then described, that is gas phase combustion models, condensed phase pyrolysis models, fire suppression models, wall functions, and heat transfer models. Despite the rapid development and completeness of these models related to fire phenomena, many limitations exist which should be always kept in mind by the users. Recommendations for CFD modeling of tunnel fires are presented.

Keywords CFD · Turbulence · Discretization · Combustion · Pyrolysis · Fire suppression · Wall function · Heat transfer · Limitation · Suggestion

17.1 Introduction

In the past several decades, CFD modeling has been rapidly developed together with significantly increased capacities of the computers.

There have been some commercial CFD tools widely used in a variety of application fields, for example, ANSYS Fluent, ANSYS CFX, PHOENICS, STAR-CCM+. Although, these general CFD tools embed many models and have strong capability of modeling different phenomena, they are generally not well tailored for fire modeling.

There have also been some specific CFD tools developed for use in fire modeling, such as JASMINE, SMARTFIRE, SOFIE, Fire Dynamics Simulator (FDS) [1], and FireFoam [2]. Among these, FDS developed by NIST [1] has become the standard in the fire community.

To date, CFD modeling has been widely used in performance-based fire safety design. Many research and application papers on CFD modeling of tunnel fires can

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be found in the literature. For example, Cheong et al. [3] simulated the burning of wood pallets, and Li et al. [4] simulated smoke characteristics of the large fires in the Runehamar tunnel fire tests carried out by Ingason et al. [5, 6].

CFD modeling simulates complex phenomena by use of numerous models. The CFD users are required to not only efficiently use the tool, but also to understand the embedded mechanisms. In this chapter, the basics of CFD modeling and the models related to fire dynamics are introduced, and limitations and recommendations are presented.

17.2 CFD Basics

The fundamental idea of CFD modeling is to divide a computation domain into a large number of small cells, and to solve a set of differential equations with sub-models using different solution algorithm. Within each cell, the properties are assumed to be uniform. The phenomena at a scale larger than the cell size are directly solved using the controlling equations but those at a smaller scale are simulated using sub-models.

17.2.1 Controlling Equations

The controlling equations describing the conservation of mass, momentum, and energy can be written as follows:

Mass:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=S_m \tag{17.1}$$

or in terms of individuals species (mass fraction Y):

$$\begin{aligned}&\frac{\partial \rho Y_i}{\partial t}+\frac{\partial(\rho u Y_i)}{\partial x}+\frac{\partial(\rho v Y_i)}{\partial y}+\frac{\partial(\rho w Y_i)}{\partial z}\\&=\frac{\partial}{\partial x}(\rho D_i \frac{\partial Y_i}{\partial x})+\frac{\partial}{\partial y}(\rho D_i \frac{\partial Y_i}{\partial y})+\frac{\partial}{\partial z}(\rho D_i \frac{\partial Y_i}{\partial z})+S_{m,i}\end{aligned} \tag{17.2}$$

Momentum:

$$\begin{aligned}&\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u u)}{\partial x}+\frac{\partial(\rho u v)}{\partial y}+\frac{\partial(\rho u w)}{\partial z}\\&=\frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x})+\frac{\partial}{\partial y}(\mu \frac{\partial u}{\partial y})+\frac{\partial}{\partial z}(\mu \frac{\partial u}{\partial z})-\frac{\partial p}{\partial x}+S_{M,x}\end{aligned} \tag{17.3}$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho uv)}{\partial x}+\frac{\partial(\rho vv)}{\partial y}+\frac{\partial(\rho vw)}{\partial z}$$
$$=\frac{\partial}{\partial x}(\mu\frac{\partial v}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial v}{\partial z})-\frac{\partial p}{\partial y}+S_{M,y} \tag{17.4}$$

$$\frac{\partial(\rho w)}{\partial t}+\frac{\partial(\rho uw)}{\partial x}+\frac{\partial(\rho vw)}{\partial y}+\frac{\partial(\rho ww)}{\partial z}$$
$$=\frac{\partial}{\partial x}(\mu\frac{\partial w}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial w}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial w}{\partial z})-\frac{\partial p}{\partial z}+S_{M,z} \tag{17.5}$$

Energy:

$$\frac{\partial(\rho h)}{\partial t}+\frac{\partial(\rho uh)}{\partial x}+\frac{\partial(\rho vh)}{\partial y}+\frac{\partial(\rho wh)}{\partial z}=\frac{\partial}{\partial x}(k\frac{\partial T}{\partial x})+\frac{\partial}{\partial y}(k\frac{\partial T}{\partial y})+\frac{\partial}{\partial z}(k\frac{\partial T}{\partial z})+S_h \tag{17.6}$$

where

$$S_m=\dot{m}'''_{net},\ S_{m,i}=\dot{m}'''_{net,i}$$

$$S_{M,x}=\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial u}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial u}{\partial z})-\frac{2}{3}\frac{\partial}{\partial x}\left[\mu(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})\right]+\rho g_x+\sum F_x$$

$$S_{M,y}=\frac{\partial}{\partial x}(\mu\frac{\partial v}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial v}{\partial z})-\frac{2}{3}\frac{\partial}{\partial y}\left[\mu(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})\right]+\rho g_y+\sum F_y$$

$$S_{M,z}=\frac{\partial}{\partial x}(\mu\frac{\partial w}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial w}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial w}{\partial z})-\frac{2}{3}\frac{\partial}{\partial z}\left[\mu(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})\right]+\rho g_z+\sum F_z$$

$$S_h=\dot{Q}'''_{net}+\Phi+\frac{\partial p}{\partial t}+u\frac{\partial p}{\partial x}+v\frac{\partial p}{\partial y}+w\frac{\partial p}{\partial z}$$

$$\Phi=\mu\left\{2[(\frac{\partial u}{\partial x})^2+(\frac{\partial v}{\partial y})^2+(\frac{\partial w}{\partial z})^2]+(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x})^2+(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x})^2+(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y})^2\right\}$$
$$-\frac{2}{3}\mu(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})^2$$

In the above equations, ρ is the density (kg/m^3), t is the time (s), x, y, z are the cartesian axis (m) and u, v, w are the velocity in the x, y, and z direction respectively (m/s). D is the mass diffusivity (m^2/s), μ is the viscosity (kg/(m s)), k is the heat conductivity (kW/(m K)), p is the pressure (Pa), g is the gravitational acceleration(m^2/s), h is the specific enthalpy (kJ/kg), S is the source term, F is the force term (N/m^3), Y is the species mass fraction and Φ is the dissipation function. Subscripts m is the mass, M is the momentum, h is the enthalpy, F is the external force such as drag exerted by water droplets, and i is the ith species. Superscript (·) indicates per unit time and ("') per unit volume.

Note that the kinetic energy has been replaced by tensors and force terms, and g is the gravity vector. The stress sensors are solved by the deformation rate of the fluid volume.

17.2.2 Equation of state

Thermodynamic equilibrium can be assumed for an ideal gas. The state equation for pressure can be expressed as:

$$p = \frac{\overline{R}}{M}\rho T \tag{17.7}$$

with ambient pressure distribution:

$$\frac{dp_o}{dz} = -\rho_o g \tag{17.8}$$

The state equation for internal energy, e, and enthalpy, h, can be written as:

$$e = c_v T \text{ and } h = c_p T \tag{17.9}$$

For gases consisting of N species, the pressure can be summed as:

$$p = \sum_{i=1}^{N} p_i = \sum_{i=1}^{N} \left(\frac{\overline{R}\rho_i T_i}{M_i}\right) \tag{17.10}$$

and the total enthalpy can be estimated by:

$$h = \sum_{i=1}^{N} \int_{T_o}^{T} c_{p,i} dT \tag{17.11}$$

In the above equations, $\overline{R}$ is the universal gas constant (8.314 kJ/(kmol K)), M is the molecular weight (kg/kmol), T is the gas temperature in Kelvin (K), e is the specific internal energy (kJ/kg), h is the enthalpy (kJ/kg), c_p is the specific heat at

constant pressure (kJ/(kg K)), c_v is the specific heat at constant volume(kJ/(kg K)), p_o is the ambient pressure (Pa) and z is the altitude height (m). Subscript i represent the ith species.

17.2.3 Turbulence

All flows are stable below a certain Reynolds number ($\mathrm{Re}=\rho ul/\mu$, l is length scale), referred to as laminar flow. However, above a certain Reynolds number, the flows become unstable and turbulent, referred to as turbulent flow. Between these regimes, the flows are called transitional flows.

There are different models that can be used in CFD simulations to simulate the turbulence. They can be primarily classified into three types, Navier–Stokes models, large eddy simulation (LES) and direct numerical simulation (DNS).

In turbulent flows, the fluctuations results in additional stresses on the fluid, called Reynold stresses. The mechanism for diffusion of momentum and energy is different between laminar and turbulent flows.

17.2.3.1 Averaged Navier–Stokes models

Averaged Navier–Stokes models solve the averaged controlling equations, and introduce sub-models to solve the terms related to fluctuating components in momentum and energy equations. The flow variables, that is, velocity and pressure, are decomposed into two components: a mean component and a fluctuating component, for example, $\varphi = \overline{\varphi} + \varphi'$. There are two averaging methods that could be used: the Reynolds averaged Navier–Stokes (RANS) model or Favre averaged Navier–Stokes (FANS) model. The Reynolds averaged method solves the time averaged controlling equations while the Favre averaged method solves the weighted averaged equations based on Reynolds averaged controlling equations. If the density fluctuations are small in some specific cases, we can obtain the same equations using both methods. Compared to RANS, FANS is much better in handling compressible flows. Here, the Favre averaged Navier–Stokes model is presented. The Favre averaging is a weighting averaging method, which is given by

$$\tilde{\varphi}(x,t) = \frac{\overline{\rho\varphi}}{\overline{\rho}} \tag{17.12}$$

where φ is a variable property. Superscript "-" indicates average value over a small time increment and "~" indicates favre averaged value.

The controlling equations in Cartesian coordinates can, therefore, be expressed as:

Mass:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial(\overline{\rho}\tilde{u})}{\partial x} + \frac{\partial(\overline{\rho}\tilde{v})}{\partial y} + \frac{\partial(\overline{\rho}\tilde{w})}{\partial z} = S_m \tag{17.13}$$

or in terms of individuals species:

$$\frac{\partial(\overline{\rho}\tilde{Y})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{Y})}{\partial x}+\frac{\partial(\overline{\rho}\tilde{v}\tilde{Y})}{\partial y}+\frac{\partial(\overline{\rho}\tilde{w}\tilde{Y})}{\partial z}=\frac{\partial}{\partial x}(\overline{\rho}D\frac{\partial\tilde{Y}}{\partial x})+\frac{\partial}{\partial y}(\overline{\rho}D\frac{\partial\tilde{Y}}{\partial y})$$
$$+\frac{\partial}{\partial z}(\overline{\rho}D\frac{\partial\tilde{Y}}{\partial z})-\left[\frac{\partial(\widetilde{\overline{\rho}u''Y''})}{\partial x}+\frac{\partial(\widetilde{\overline{\rho}v''Y''})}{\partial y}+\frac{\partial(\widetilde{\overline{\rho}w''Y''})}{\partial z}\right]+\tilde{S}_{m,Y} \tag{17.14}$$

Momentum:

X axis:

$$\frac{\partial(\overline{\rho}\tilde{u})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{u})}{\partial x}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{v})}{\partial y}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{w})}{\partial z}=\frac{\partial}{\partial x}(\mu\frac{\partial\tilde{u}}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial\tilde{u}}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial\tilde{u}}{\partial z})$$
$$-\frac{\partial\tilde{p}}{\partial x}-\left[\frac{\partial(\widetilde{\overline{\rho}u''^2})}{\partial x}+\frac{\partial(\widetilde{\overline{\rho}u''v''})}{\partial y}+\frac{\partial(\widetilde{\overline{\rho}u''w''})}{\partial z}\right]+\tilde{S}_{M,x} \tag{17.15}$$

Y axis:

$$\frac{\partial(\overline{\rho}\tilde{v})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{v})}{\partial x}+\frac{\partial(\overline{\rho}\tilde{v}\tilde{v})}{\partial y}+\frac{\partial(\overline{\rho}\tilde{v}\tilde{w})}{\partial z}=\frac{\partial}{\partial x}(\mu\frac{\partial\tilde{v}}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial\tilde{v}}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial\tilde{v}}{\partial z})$$
$$-\frac{\partial\tilde{p}}{\partial y}-\left[\frac{\partial(\widetilde{\overline{\rho}u''v''})}{\partial x}+\frac{\partial(\widetilde{\overline{\rho}v''^2})}{\partial y}+\frac{\partial(\widetilde{\overline{\rho}v''w''})}{\partial z}\right]+\tilde{S}_{M,y} \tag{17.16}$$

Z axis:

$$\frac{\partial(\overline{\rho}\tilde{w})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{w})}{\partial x}+\frac{\partial(\overline{\rho}\tilde{v}\tilde{w})}{\partial y}+\frac{\partial(\overline{\rho}\tilde{w}\tilde{w})}{\partial z}=\frac{\partial}{\partial x}(\mu\frac{\partial\tilde{w}}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial\tilde{w}}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial\tilde{w}}{\partial z})$$
$$-\frac{\partial\tilde{p}}{\partial z}-\left[\frac{\partial(\widetilde{\overline{\rho}u''w''})}{\partial x}+\frac{\partial(\widetilde{\overline{\rho}v''w''})}{\partial y}+\frac{\partial(\widetilde{\overline{\rho}w''^2})}{\partial z}\right]+\tilde{S}_{M,z} \tag{17.17}$$

Energy:

$$\frac{\partial(\overline{\rho}\tilde{h})}{\partial t}+\frac{\partial(\overline{\rho}\tilde{u}\tilde{h})}{\partial x}+\frac{\partial(\overline{\rho}\tilde{v}\tilde{h})}{\partial y}+\frac{\partial(\overline{\rho}\tilde{w}\tilde{h})}{\partial z}=\frac{\partial}{\partial x}(k\frac{\partial\tilde{T}}{\partial x})+\frac{\partial}{\partial y}(k\frac{\partial\tilde{T}}{\partial y})+\frac{\partial}{\partial z}(k\frac{\partial\tilde{T}}{\partial z})$$
$$-\left[\frac{\partial(\widetilde{\overline{\rho}u''h''})}{\partial x}+\frac{\partial(\widetilde{\overline{\rho}v''h''})}{\partial y}+\frac{\partial(\widetilde{\overline{\rho}w''h''})}{\partial z}\right]+\tilde{S}_{h} \tag{17.18}$$

Note that the main difference between the above equations for turbulent flows and for laminar flows is the presence of additional terms on the right-hand sides of the momentum equations Eqs. (17.15–17.17), the species transport equation Eq. (17.14) and the energy equation Eq. (17.18). These terms indicate the additional diffusion of momentum and mass, and extra dissipation of energy. The terms in the momentum equation are called the Reynolds stress and therefore, the momentum equations are called the Reynolds equations. The Navier–Stokes turbulence models are proposed to correlate these turbulent terms with the mean values of the flows. The source terms can be easily obtained by averaging the original terms.

The averaged Navier–Stokes turbulence models mainly include: the zero equation model (mixing length model), two equation k-ε model, Reynolds stress equation model, and algebraic stress model. The most widely used and validated standard *k-ε* model is briefly depicted here.

The turbulent kinetic energy, K (m^2/s^2), and viscous dissipation rate, ε (m^2/s^3), respectively are defined as:

$$K = \frac{1}{2}\widetilde{u_i' u_i'} = \frac{1}{2}(\widetilde{u'^2} + \widetilde{v'^2} + \widetilde{w'^2}),\ \varepsilon = \frac{\mu_t}{\bar{\rho}}\widetilde{\frac{\partial u_i'}{\partial x_j}\cdot\frac{\partial u_i'}{\partial x_j}},\ i,\ j = 1,\ 2,\ 3 \tag{17.19}$$

where μ_t is the turbulent viscosity (kg/(m s)), which is assumed to be isotropic in the *k-ε* model. u', v', and w' are the fluctuating component of velocity u, v, and w respectively (m/s). Subscripts i and j indicate x (1), y (2), or z (3) axis.

The Reynolds stress in the momentum equation, τ_{ij} (kg/(m s^2)), is linked to the mean rates of deformation by:

$$\tau_{ij} = -\bar{\rho}\widetilde{u_i' u_j'} = \mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\left(\mu_t \frac{\partial \tilde{u}_i}{\partial x_j} + \bar{\rho}K\right)\delta_{ij} \tag{17.20}$$

where the Kronecker delta, $\delta_{i,j}$, is defined as:

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \quad i,\ j = 1,\ 2,\ 3 \tag{17.21}$$

Note that the turbulent terms in the momentum equation have been correlated with the mean terms. The main task left is to estimate the turbulent viscosity, μ_t. In the standard *k-ε* model, it is assumed that the turbulent eddy viscosity is proportional to the turbulent velocity scale and length scale which can be replaced by the turbulent kinetic energy and viscous dissipation rate. This assumption leads to:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{17.22}$$

The k equation can be expressed as:

$$\frac{\partial(\bar{\rho}K)}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j K)}{\partial x_j}=\frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_k}\frac{\partial K}{\partial x_j})+\mu_t\frac{\partial\tilde{u}_i}{\partial x_j}(\frac{\partial\tilde{u}_i}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_i})-\frac{2}{3}\frac{\partial\tilde{u}_i}{\partial x_j}(\mu_t\frac{\partial\tilde{u}_i}{\partial x_j}+\bar{\rho}K)\delta_{ij}-\bar{\rho}\varepsilon \tag{17.23}$$

And the ε equation can be expressed as:

$$\begin{aligned}&\frac{\partial(\bar{\rho}\varepsilon)}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j\varepsilon)}{\partial x_j}=\frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial x_j})\\&+C_{\varepsilon 1}\frac{\varepsilon}{K}\left[\mu_t\frac{\partial\tilde{u}_i}{\partial x_j}(\frac{\partial\tilde{u}_i}{\partial x_j}+\frac{\partial\tilde{u}_j}{\partial x_i})-\frac{2}{3}\frac{\partial\tilde{u}_i}{\partial x_j}(\mu_t\frac{\partial\tilde{u}_i}{\partial x_j}+\bar{\rho}K)\delta_{ij}\right]-C_{\varepsilon 2}\bar{\rho}\frac{\varepsilon^2}{K}\end{aligned} \tag{17.24}$$

where

$$C_\mu=0.09,\ C_{\varepsilon 1}=1.44,\ C_{\varepsilon 2}=1.92,\ \sigma_{\mathrm{k}}=1.0,\ \sigma_\varepsilon=1.30$$

The turbulent terms in other equations are directly correlated with the turbulent viscosity by analogy. The turbulent terms in energy equation can be expressed as:

$$-\bar{\rho}\widetilde{u_i'h}=k_t\frac{\partial\tilde{h}}{\partial x_i} \tag{17.25}$$

The turbulent terms in species scalar equation is expressed as:

$$-\bar{\rho}\widetilde{u_i'Y}=(\rho D)_t\frac{\partial\tilde{Y}}{\partial x_i} \tag{17.26}$$

The corresponding turbulent conductivity, k_t, can be estimated by:

$$k_t=\frac{\mu_t}{\mathrm{Pr}_t} \tag{17.27}$$

And the turbulent mass diffusivity, $(\rho D)_t$, is:

$$(\rho D)_t=\frac{\mu_t}{\mathrm{Sc}_t} \tag{17.28}$$

where Pr_t is turbulent Prandtl number and Sc_t is turbulent Schdmit number. It should be kept in mind that the standard k-ε model is only suitable for flows with high Reynolds numbers, that is turbulent flows. There are also k-ε equations for low Reynold numbers where the viscous diffusivity term needs to be accounted for.

17.2.3.2 Large Eddy Simulation (LES)

As described in the last section, RANS introduces extra equations to model the turbulence, and both large and small eddies are modeled using turbulence sub-models. In contrast, LES directly simulates the mean flow and the largest eddies and only simulate the small eddies using sub-grid scale models. LES models can use explicit filter functions to filter the small eddies. The spatial filtering operation could be expressed as follows:

$$\hat{\varphi}(x,t) = \int_{\Delta} \varphi(r,t) G(|x-r|) dr \tag{17.29}$$

where G is the filter function and Δ is the filter width which is generally equal to the cell size. The most common filter functions include: the Top hat filter function, the Gaussian filter function, and the Fourier Cut-Off filter function [7].

Similar to the Navier–Stokes turbulent models, the Favre averaging is used here, which is given by

$$\tilde{\varphi}(x,t) = \frac{\widehat{\rho\varphi}}{\hat{\rho}} \tag{17.30}$$

The controlling equations for large eddy simulation are similar to those for the FANS model except the turbulent stress terms:

Mass:

$$\frac{\partial \hat{\rho}}{\partial t} + \frac{\partial(\hat{\rho}\tilde{u}_j)}{\partial x_j} = S_m \tag{17.31}$$

or in terms of individuals species:

$$\frac{\partial(\hat{\rho}\tilde{Y})}{\partial t} + \frac{\partial(\hat{\rho}\tilde{u}_j\tilde{Y})}{\partial x_j} = \frac{\partial}{\partial x_j}(\hat{\rho}D\frac{\partial \tilde{Y}_j}{\partial x_j}) - \frac{\partial}{\partial x}(\widehat{\rho u_j Y} - \hat{\rho}\tilde{u}_j\tilde{Y}) + \tilde{S}_{m,Y} \tag{17.32}$$

Momentum:

$$\frac{\partial(\hat{\rho}\tilde{u})}{\partial t} + \frac{\partial(\hat{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial}{\partial x}\left[\tilde{p}\delta_{ij} - \mu_t\frac{\partial \tilde{u}_i}{\partial x_j}(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}) + \frac{2}{3}(\mu_t\frac{\partial \tilde{u}_i}{\partial x_j})\delta_{ij}\right] - \frac{\partial(\widehat{\rho u_i u_j} - \hat{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} + S_{M,i} \tag{17.33}$$

Energy:

$$\frac{\partial(\hat{\rho}\tilde{h})}{\partial t} + \frac{\partial(\hat{\rho}\tilde{u}_j\tilde{h})}{\partial x_j} = \frac{\partial}{\partial x_j}(\frac{k}{c_p}\frac{\partial \tilde{h}}{\partial x_j}) - \frac{\partial}{\partial x}(\widehat{\rho u_j h} - \hat{\rho}\tilde{u}_j\tilde{h}) + \tilde{S}_h \tag{17.34}$$

It should be kept in mind that all the variables are filtered values. Also, note that the turbulent stress terms in the controlling equations for LES are different with the Reynolds stress terms for FANS owing to the different definitions. Despite the difference, the turbulent stresses also need to be solved using sub grid scale (SGS) models. The commonly used SGS models mainly include the Smagorinsky model, structure function model, mixed scale model, dynamic SGS models, and one-equation SGS models [7]. Here, the basic Smagorinsky model which is used in FDS [1] is depicted briefly.

In the Smagorinsky model, the turbulent eddies are assumed to be isotropic. The subgrid turbulent stresses are modeled as:

$$\tau_{ij} = \widehat{\rho u_i u_j} - \hat{\rho}\tilde{u}_i\tilde{u}_j = -2\mu_{SGS}\tilde{S}_{ij} \tag{17.35}$$

where the rate-of-strain tensor, $\tilde{S}_{ij}$, is defined as:

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial\tilde{u}_n}{\partial x_n}\delta_{ij}, \quad n = 1,\ 2,\ 3 \tag{17.36}$$

It is assumed that the turbulent viscosity can be described in terms of a length scale and the average strain rate of the flow, which suggests:

$$\mu_{SGS} = \rho(C_s\Delta)^2\left[2\tilde{S}_{ij}\cdot\tilde{S}_{ij} - \frac{2}{3}\left(\frac{\partial\tilde{u}_n}{\partial x_n}\right)^2\right]^{\frac{1}{2}} \tag{17.37}$$

where C_s is a coefficient ranging between 0.065 and 0.3. This value is set to 0.2 in FDS [1].

Similar to the Favre averaged Navier–Stokes models, the turbulent terms in other equations are also correlated with the turbulent viscosity by analogy. The turbulent terms in energy equation can be expressed as:

$$\widehat{\rho u_i h} - \hat{\rho}\tilde{u}_i\tilde{h} = -k_{SGS}\frac{\partial\tilde{T}}{\partial x_j} \tag{17.38}$$

The turbulent terms in scalar equation is expressed as:

$$\widehat{\rho u_i Y} - \hat{\rho}\tilde{u}_i\tilde{Y} = -(\rho D)_{SGS}\frac{\partial\hat{Y}}{\partial x_j} \tag{17.39}$$

The corresponding turbulent conductivity and mass diffusivity can be simply estimated by:

$$k_{SGS} = \frac{\mu_{SGS}c_p}{\mathrm{Pr}_{SGS}} \tag{17.40}$$

and

$$(\rho D)_{SGS} = \frac{\mu_{SGS}}{\mathrm{Sc}_{SGS}} \tag{17.41}$$

In FDS, both the turbulent Prandtl number and the Schmidt number are set to be 0.5.

17.2.3.3 Direct Numerical Simulation

Direct numerical simulation (DNS) directly solves the controlling equations and directly simulates both the largest and smallest eddies. Note that the controlling equations for DNS are the same as the equations for laminar flows. Therefore, the mesh size should be smaller than the smallest eddy in the flow, where the Reynolds number is equivalent to unity. The grid number in three-dimensional simulations scales as 9/4 power of the Reynold number. As the Reynolds number increases, the difference between the smallest and largest eddies also increases, and the required grid numbers increases rapidly. Although, some investigations suggest that a reduction by a factor of 100 in the number of the cells is possible without significant loss of accuracy, it is apparent that a DNS calculation is very costly.

Note that use of DNS only suggests the possibility of modeling the flow perfectly, rather than modeling the fire-induced flows perfectly since, the later depends not only the flow models but the other sub-models which will be discussed later.

17.2.4 Discretization Methods

The controlling equations need to be discretized and solved over the cells. Three discretization methods are widely used, that is: the finite volume method (FVM), finite element method (FEM) and finite difference method (FDM). Additionally, the boundary element method, spectral element method, and other high-resolution discretization schemes could be used. Here, we focus on the finite volume method which is widely used in computational fluid dynamics owing to its clear physical meaning and completeness. First we discretize a computation domain into a large amount of small control volumes.

Note that the controlling equations for mass, momentum, and energy can be written in a simple form:

$$\frac{\partial(\rho\varphi)}{\partial t} + div(\rho\varphi\mathbf{u}) = div(\Gamma grad(\varphi)) + S \tag{17.42}$$

where φ is a variable property (1 for mass, u for momentum and h for energy), u is the velocity vector and S is a source term. The symbol *div* is the divergence and *grad* is the gradient.

Integrating the above equation from time t to $t+\Delta t$ for the control volume (CV) suggests:

$$\int_{CV}\int_{t}^{t+\Delta t}\frac{\partial(\rho\varphi)}{\partial t}dtdV+\int_{CV}\int_{t}^{t+\Delta t}div(\rho\varphi\mathbf{u})dtdV$$
$$=\int_{CV}\int_{t}^{t+\Delta t}div(\Gamma grad(\varphi))dtdV+\int_{CV}\int_{t}^{t+\Delta t}SdtdV \tag{17.43}$$

17.2.4.1 Temporal Discretization

The integration of the terms in the above equation, except the first term on the left-hand side signifying the rate of change, from time to t+ Δt can be expressed in such a way:

$$\int_{t}^{t+\Delta t}\varphi dt=\Delta t\left[\xi\varphi(t+\Delta t)+(1-\xi)\varphi(t)\right] \tag{17.44}$$

where Δt is time step (s) and ξ is a coefficient for the discretization.

If $\xi=0$, the term φ at time $t+\Delta t$ is estimated fully based on the values at time t, and the resulting scheme is called fully explicit or Euler explicit scheme. If $\xi=1$, the term φ at time t+Δt is estimated fully based on the values at time $t+\Delta t$, and the resulting scheme is called fully implicit or Euler implicit scheme. If $\xi=1/2$, the scheme is called the Crank–Nicolson scheme. However, note that the first term in Eq. (17.43) signifying the rate of change includes the derivative of time and the time increment can be depleted, and thus it always has the same form, regardless of the schemes.

For fully explicit scheme, stability conditions, that is, Courant–Friedrichs–Lewy (CFL) condition and Von Neumann criterion, need to be fulfilled to avoid instability.

For structured grids, the CFL condition can be simply expressed as:

$$\Delta t\max(\frac{|u|}{\Delta x},\frac{|v|}{\Delta y},\frac{|w|}{\Delta z})<1 \tag{17.45}$$

and the Von Neumann criterion is:

$$\Delta t\max(D,v,a)(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})<\frac{1}{2} \tag{17.46}$$

where Δx, Δy, Δz are the size of the grid cell in the x, y, and z direction respectively, D is the mass diffusivity (m^2/s), v is the kinematic viscosity (m^2/s) and a is the thermal diffusivity (m^2/s).

These limitations are used to stabilize the solution by forcing the coefficients in the numerical equations above zero. The physical meaning is to avoid the flow of mass, momentum, and energy transferring too fast.

A fully implicit scheme indicates that the obtained results are always stable in theory. However, small time steps are required to reduce computation errors since the accuracy of the fully implicit scheme is generally first order or second order in time. For example, the fully implicit Euler scheme is only first order. Further, small time steps could also be required in case of a transient flow involving time dependent boundaries or very complicated phenomena.

17.2.4.2 Spatial Discretization

For the convection term and the diffusion terms, we need to discretize the term as a derivative of the volume size. Let us consider, a control volume enclosed by two neighboring volume west (W) and east (E) and the two corresponding boundaries are called *w* and *e* (*x* axis from w to e).

$$\int_{CV} \frac{\partial \varphi}{\partial x} dV = (\Delta y \Delta z)(\varphi_e - \varphi_w) \tag{17.47}$$

The values at the boundaries need to be replaced using the values of the cells beside the control volume. There are many schemes for discretization of the boundary terms, including: the central differencing scheme, upwind differencing scheme, hybrid differencing scheme, power-law scheme, QUICK scheme, and other high order schemes, for example the Superbee scheme for convection [8].

The central differencing scheme for this volume can be expressed as:

$$\varphi_w = \frac{\varphi_W + \varphi_{CV}}{2} \text{ and } \varphi_e = \frac{\varphi_{CV} + \varphi_E}{2} \tag{17.48}$$

For a convection and diffusion problem, the central differencing scheme may result in instability unless it fulfills the condition for the Peclet number:

$$Pe = \frac{\rho u}{\Gamma \Delta x} < 2 \tag{17.49}$$

The physical meaning is that the directionality of influencing is not expressed well using the central differencing scheme in a flow.

The upwind scheme suggests that the value of the upwind mesh is used as the boundary value, for example, if the wind is from west to east, we have

$$\varphi_w = \varphi_W \text{ and } \varphi_e = \varphi_{CV} \tag{17.50}$$

Although the upwind scheme is so simple and its accuracy is only first order, it is useful for convection problems. To increase accuracy at a high *Pe* number, the hybrid differencing scheme of Spalding can be used. The hybrid differencing scheme is a combination of the upwind scheme and central differencing scheme, and is valid for the whole range of the Peclet number.

The accuracy of hybrid and upwind schemes is only first order. Higher order differencing schemes could be used to speed up the computation. The quadratic upwind differencing scheme (QUICK) [9] is a good example:

$$\varphi_w = \frac{6}{8}\varphi_P + \frac{3}{8}\varphi_W - \frac{1}{8}\varphi_E \text{ and } \varphi_e = \frac{6}{8}\varphi_E + \frac{3}{8}\varphi_P - \frac{1}{8}\varphi_{EE} \tag{17.51}$$

where *EE* is the further east mesh.

17.2.5 Solution Algorithms

After the discretization of the equations we can obtain several discretized equations for each mesh. To solve these large numbers of algebraic equations, special algorithms need to be applied. The core of the solution is to solve the momentum equation.

Solution algorithms include the full coupling method and the pressure–velocity linkage method. The full coupling method solves the system of all the algebraic equations. The problem is that the system is highly nonlinear. Therefore, the full coupling method is much less efficient compared to the pressure–velocity coupling method. Most commercial CFD software only adopts the pressure–velocity linkage method.

The pressure–velocity linkage method could be divided into two sets, the pressure-based methods and the density-based methods. The pressure-based methods are more often used in incompressible flows while the density-based methods in compressible flows. The pressure-based methods can be classified into: the SIMPLE-based algorithms and the Poisson algorithms. The SIMPLE-based algorithms include SIMPLE, SIMPLER, SIMPLEC, and PISO. They calculate the pressure on the staggered grid arrangement following a guess-and-correct procedure. The SIMPLER algorithm is more efficient at correcting the pressure than the SIMPLE algorithm and thus regarded as the standard algorithm in many CFD codes. The Poisson algorithms consist of, for example,the Marker-And-Cell (MAC) method [10], the simplified MAC method SMAC [11], and ALE [12]. These direct-solve the Poisson equation for the pressure and show high efficiency. However, the SIMPLE-based methods are more widely used in the general CFD codes.

17.3 Sub-Models Related to Tunnel Fires

17.3.1 Gas Phase Combustion

The gas-phase combustion theoretically, always takes a discrete amount of time. However, compared to the flow time the reaction time can generally be ignored. The Damköhler number is used to characterize these two times [13, 14]:

$$D_a = \frac{t_{turbulent}}{t_{combustion}} \tag{17.52}$$

We may classify the gas phase combustion models in two ways, that is: the *generalized finite rate combustion* and *infinite rate conserved scalar combustion*.

The generalized finite rate combustion model requires accurate modeling of the diffusion of fuel and oxygen, which accordingly requires very fine meshes and small time steps. The generalized finite rate combustion model includes the laminar finite rate chemistry model, the eddy breakup and dissipation model, etc. [7, 15]. The finite rate chemistry model uses the Arrhenius kinetic expression for the reaction rate. The eddy breakup and dissipation models assume that the local strain rate of turbulence dominates the reaction rate in turbulent flames. The eddy breakup reaction rate is taken to be simply based on the species concentration fluctuations and the rate of eddy breakup.

The conserved scalar combustion models have no chemical source terms in the scalar equations due to the introduction of a mixture fraction. Such models includes: the infinite rate mixture fraction model, the laminar flamelet model, the probability density function model, etc. The infinite rate mixture fraction model assumes that the reaction of fuel and oxygen completes immediately after mixing. The laminar flamelet model considers a flame as an ensemble of laminar flamelets. The probability density function model applies the probability function to account for the interaction between the turbulence and the combustion.

For CFD modeling of a tunnel fire, the computation domain is very large compared to the dimensions of the fire source. A finite rate combustion model requires very fine grid sizes and small time steps for modeling of the fire domain, which suggests that modeling of a flame using the finite rate method and modeling of smoke movement in a tunnel are at different scales and the finite rate combustion models are not particularly suitable for use in engineering applications at present. Instead, the infinite rate mixture fraction model is more practical and has already been widely used in modeling of tunnel fires. The mixture fraction model used in FDS [1] is briefly described below.

The chemistry equation is assumed to be:

$$v_F \text{ Fuel} + vo\,\text{O}_2 \rightarrow \sum_i v_{P,i} \text{ Products} \tag{17.53}$$

Thus

$$\frac{\dot{m}_F'''}{v_F M_F} = \frac{\dot{m}_O'''}{v_O M_O} \tag{17.54}$$

The mixture fraction, Z, is defined as:

$$Z = \frac{sY_F - (Y_O - Y_O^\infty)}{sY_F^I + Y_O^\infty} \tag{17.55}$$

where

$$s = \frac{v_O M_O}{v_F M_F}$$

Mass conservation:

$$\rho \frac{DZ}{Dt} = \nabla \cdot \rho D \nabla Z \tag{17.56}$$

Define the flame surface as:

$$Z(x,t) = Z_f = \frac{Y_O^\infty}{sY_F^I + Y_O^\infty} \tag{17.57}$$

The conditions for the flame surface:

$$Y_O(Z) = \begin{cases} Y_O^\infty (1 - Z / Z_f) & Z < Z_f \\ 0 & Z > Z_f \end{cases} \tag{17.58}$$

In the above equations, v_F, v_O, and v_p are the stoichiometric coefficient for the fuel, oxygen, and combustion products, $\dot{m}'''$ is a mass source term (kg/(m^3 s)), M is the molecular weight (kg/kmol), Y is the fuel mass fraction in the volume, Z is the mixture fraction. Subscript F is the fuel, f is the flame, O is the oxygen, and P is the combustion product. Superscript ∞ indicates ambient condition and I indicates inlet.

The mixture fraction model has proven to be simple and robust, and coarse meshes are allowed, however, the flammability conditions are difficult to determine in the coarse meshes.

17.3.2 Condensed Phase Pyrolysis

In most engineering applications, we simply simulate a tunnel fire using a gas burner producing a fixed heat release rate (HRR) or a HRR curve. Therefore, only gas combustion is simulated.

In some cases, modeling of a pool fire or a solid fire may also be of some interest. For example, to investigate the performance of a fire suppression system using CFD, a pool fire or a more realistic solid fire generally needs to be modeled. Unfortunately, the present capability of CFD tools seldom succeeds in these tasks due to lack of understanding of mechanisms of these condensed phase pyrolysis. Here, only a short description of the pyrolysis models is presented for information only.

17.3.2.1 Solid Phase

The pyrolysis rate of a solid fuel is mainly related to the fuel temperature and mass concentration and could be correlated with the Arrhenius expression [16, 17] for a small volume inside the fuel:

$$\frac{dY_f}{dt} = -A_{pef} Y_f \exp(-\frac{E_A}{RT_f}) \tag{17.59}$$

where Y_f is the fuel mass fraction, T_f is the fuel temperature (K), A_{pef} is the preexponential factor (pef), and E_A is the activation energy (kJ/kmol). Both the activation energy and the preexponential factor are generally considered as constant for a specific fuel, and could be obtained from small-scale tests.

Heat conduction inside the fuel needs to be appropriately modeled. The heat is absorbed by the fuel surfaces and conducted into the fuel to support the pyrolysis. The fuel vapor evaporates, penetrates to the surface, mixes with oxygen and burns in the air. Note that for thermoplastic materials the mechanism of heat transfer into the fuels is slightly different.

17.3.2.2 Liquid Phase

The volume fraction of the vapor right above the surface of a liquid pool or a liquid droplet can be estimated according to the Clausius–Clapeyron relation as follows [18]:

$$X_f = \exp\left[-\frac{L_v M_f}{R}(\frac{1}{T_s} - \frac{1}{T_b})\right] \tag{17.60}$$

where T_s is the liquid surface temperature (K), T_b is the boiling temperature (K), L_v is the heat of vaporization (kJ/kg) and X_f is the volume fraction of fuel vapour. The produced fuel vapour leaves the fuel surface, mixes with air and burns. By comparing the difference between the estimated fuel vapour concentration, according to the Clausius–Clapeyron relation and the actual volume fraction of fuel vapor above the fuel surface the mass burning rate could be estimated. It can be expected from the above equation that the fuel evaporation rate is very sensitive to the surface temperature. The movement of liquid fuels is at a much smaller scale and difficult to model.

17.3.3 Fire Suppression

Recently, the interest in using water-based fire suppression systems in tunnels has increased significantly. For modeling of fire suppression in tunnels, generally a solid fire is required to be modeled. However, as discussed previously, the current CFD

technique cannot model the condensed phase pyrolysis well. Similarly, fire suppression in tunnels cannot be modeled well. Nonetheless, the basic theory related to water-based fire suppression is illustrated here and can be useful on occasion.

The water droplets are discharged into the tunnel, exchanges momentum and heat with the hot gases in the air, and on the fuel surfaces. All these processes need to be modeled. At a very short distance after the water is discharged from a nozzle, it is transformed into a large number of small droplets with different sizes. The cumulative volume distribution of the water droplets can be expressed as: [28]

$$F_v(d) = \begin{cases} \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_0^D \frac{1}{\sigma d'} \exp\left(-\frac{[\ln(d'/d_m)]^2}{2\sigma^2}\right) dd', & d \le d_m \\ 1 - \exp[-0.693(\dfrac{d}{d_m})^{\gamma}], & d > d_m \end{cases} \tag{17.61}$$

where d is the water droplet diameter (m), d_m is the median volumetric droplet diameter corresponding to half the mass (m), γ and σ are the empirical constants equal to approximately 2.4 and 0.6, respectively. The median water droplet diameter depends on the characteristics of the nozzle, see Sect. 18.6.4.

Note that a water spray consists of millions of droplets with different sizes. In CFD modeling, only a limited number of water droplets with different sizes can be modeled to represent the characteristics of all the water droplets discharged from one nozzle. This simplification can cause some errors especially when only a very small amount of droplets are modeled. The water droplets discharged into the tunnel exchange mass, momentum, and energy with the hot gases. The controlling equations for the water droplets are described in Sect. 18.6.1.

For fire suppression modeling, the extinction criteria adopted play the key role. The theory of fire suppression has been described in detail in Chap. 16. There are two extinction mechanisms: gas phase extinction and condensed phase extinction. For gas phase extinction, Eq. (16.12) can be applied. In FDS, the same model is used but the effect of water is neglected. Another choice is to use the model proposed by Willians [13] although its use relies on accurate modeling of the finite rate gas phase combustion. The interaction between the water droplets and fuel surfaces is the key mechanism of fire suppression in tunnels. However, the models available for the condensed phase extinction are too empirical. For example, FDS adopts the simple model for fire suppression proposed by Yu et al. [19]. The local HRR per unit area, $\dot{q}''(t)$, is expressed in the form [1]:

$$\dot{q}''(t) = \dot{q}_0''(t)\, \mathrm{e}^{-\int k(t)dt} \tag{17.62}$$

where the coefficient *k(t)* is expressed as:

$$k(t) = a\dot{m}_w''(t)$$

In the above equation, $\dot{q}_0''(t)$ is the HRR per unit area when no water is applied (kW/m^2), $\dot{m}_w''$ is the water density (mm/min), and a is an empirical coefficient that is dependent on the material properties of the solid fuel and its geometrical configuration.

17.3.4 Wall Function

The tunnel wall results in the main pressure loss in normal ventilation, which is also the key source for the pressure loss in fire ventilation. It is also a key boundary for the tunnel flows, which makes the tunnel fires differ from the other enclosure fires. Note that the shear stress and heat transfer at the boundary layer could be solved reasonably well only using very fine grids. In most cases, sub-models are used for modeling of the near-wall region.

A dimensionless wall-normal distance, y^+, is defined first:

$$y^+ = \frac{\rho u^* y}{\mu} \tag{17.63}$$

where $u^* = \sqrt{\tau_w / \rho}$ (m/s) is the friction velocity, y is the wall-normal distance (m) and τ_w is wall stress (N/m^2). As discussed in Chap. 10, the boundary layer consists of three sublayers, that is, the viscous sublayer, the buffer layer and the log layer. The buffer layer lies between the viscous layer and log layer, however, it is generally incorporated into the other two layers in the wall function. At the viscous sublayer, that is, $y^+ < 11.63$, the viscous force dominates and the velocity can be obtained [20]:

$$\frac{u}{u^*} = y^+ \tag{17.64}$$

At the log layer, that is, $11.63 < y^+ < 500$, the velocity can be expressed as:

$$\frac{u}{u^*} = 2.4 \ln(9.8 y^+) \tag{17.65}$$

The shearing stress at the wall can be obtained from estimation of the parameter, u/u^*. For rough tunnel walls, the roughness can easily disrupt the viscous sublayer, and thus its effect needs to be accounted for. In such cases, the coefficient of 9.8 is usually reduced and an appropriate value needs to be set for it. More information can be found in the references [21, 22].

17.3.5 Heat Transfer

17.3.5.1 Convective Heat Transfer

According to the Reynolds' analogy, similar treatment can be made for the heat transfer to the wall. Launder and Spalding [23] found that the convective heat flux at the wall exposed to air flow at high Reynolds number, $\dot{q}_c''$ (kW/m^2), can be correlated with the local parameters as follows:

$$\frac{(T_p - T_w)\rho c_p \sqrt{\tau_w / \rho}}{\dot{q}_c''} = \mathrm{Pr}_t \left[\frac{u}{u^*} + P\left(\frac{\mathrm{Pr}}{\mathrm{Pr}_t}\right) \right] \tag{17.66}$$

where T_p is the temperature at near wall point p (K), T_w is the wall temperature (K), Pr is the Prandtl number and Pr_t is the turbulent Prandtl number (0.85 for most non-metallic fluids [24]). The function P is called "pee-function", a correction function dependent on the ratio of the two Prandtl numbers. In reality, the above equation is another form of the Reynold analogy. Similar models can be found in the literature, for example, reference [25].

Another method could be to use the convective heat transfer coefficient equations directly, regardless of near-wall parameters, for example, the model used in FDS [1]. This simplified method could result in large error in modeling of a large tunnel fire, as pointed out by Li et al. [4].

17.3.5.2 Radiation Heat Transfer

The radiation transport equation (RTE) could be written in the following form:

$$\begin{aligned} \mathbf{s} \cdot \nabla I_\lambda(\mathbf{r}, \mathbf{s}) = & -\left[\kappa(\mathbf{r}, \lambda) + \sigma_s(\mathrm{r}, \lambda)\right] I_\lambda(\mathbf{r}, \mathbf{s}) + \kappa(\mathbf{r}, \lambda) I_b(\mathbf{r}, \lambda) \\ & + \frac{\sigma_s(\mathbf{r}, \lambda)}{4\pi} \int_{4\pi} \psi(\mathbf{s}, \mathbf{s}') I_\lambda(\mathbf{r}, \mathbf{s}') d\Omega \end{aligned} \tag{17.67}$$

where I is the radiation intensity radiation intensity (kW/(m^2·steradian)), $\mathbf{r}$ is a positionvector (m), $\mathbf{s}$ is a direction vector (m), s' is the scattering direction vector (m), κ is an absorption coefficient (1/m), σ_s is the scattering coefficient (1/m), Ψ is the probability that incident radiation in the direction s will be scattered into the increment of solid angle $d\Omega$ Subscript λ indicates wavelength, b indicates blackbody.

Generally we may ignore the scattering effect and assume the smoke is gray gas. The absorption coefficient of the gas needs to be estimated based on the local mass fraction of the smoke and combustion products, see Chap. 10. Note that a tunnel fire generally produces a large amount of smoke particles which dominates the total absorption coefficient rather than CO_2 and H_2O. Further, note that the soot absorbs

heat continuously, independent of the wavelengths. Therefore, generally it could be quite reasonable to simplify the description to one band model and the assumption of gray gas is quite reasonable in most cases.

At the wall surface, the incident heat flux can be expressed as:

$$\dot{q}''_{w,in}(x) = \int_{2\pi} I(x,s)ds = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi/2} I_{w,in}(\theta,\phi)\cos\theta\sin\theta d\theta d\phi \tag{17.68}$$

and the total outgoing heat flux can be expressed as:

$$\dot{q}''_{w,out}(x) = \varepsilon_w \sigma T_w^4 + (1-\varepsilon_w)\dot{q}''_{w,in}(x) \tag{17.69}$$

where θ is the angle between the incident radiation and the normal line of the wall (radian), φ is the angle between the projection incident radiation line on the surface and a reference line (radian), and ε_w is the wall emissivity.

Different radiation models may be used, primarily including: the P-1 radiation model, the Discrete Ordinates Model, the Finite Volume Method model, the Discrete Transfer Radiative Model, and the Monte Carlo model with the computation cost increasing gradually.

The P-1 radiation model uses the first-order spherical harmonic approximation. It is accurate for optically thick or dense cases, however, not accurate for optically thin cases where the high order differential approximation is required to improve the accuracy.

The discrete ordinates model discretizes the entire solid angle using a finite number of ordinate directions with weight factors. The discretized equation can be obtained by integrating over a control volume, and the edge fluxes of the control volume can be correlated with the fluxes at the volume center by the spatially weighted approximation.

The finite volume method model is quite similar to the discrete ordinates model. The discretized equation is obtained by integrating the differential equation over the control volume and solid angle. By applying the Gauss' divergence theorem, the intensity derivative term is transformed to a surface integral over all surfaces of the volume. The idea of the upwind scheme can be used in solution that the marching direction depends on the main propagation direction of the radiation intensity.

The Discrete Transfer Radiative Model is principally based on the concept of solving radiation rays in an enclosure. The radiation rays are solved along the paths between the walls. The wall surfaces can be divided into many elements. For each surface element, the solid angle is preliminarily divided into a finite number of angles and the outgoing intensity is assumed to be constant within any given angle. The governing equation, having a form similar to Beer's law, is used to obtain the outgoing intensity immediately.

The Monte Carlo model is essentially a statistical method and it attains its name from many different statistical approaches. The model simulates a finite number of photon histories by use of a random number generator to randomly determine the

emission location and direction to produce probabilistic distributions for the traveling distance.

In summary, the P-1 model is the basic model that can produce accurate results for optically dense cases, however, for both dense and thin cases the other models may need to be used. The discrete ordinates method and the finite volume method are quite similar to each other and with the same order of accuracy. The discrete transfer radiative and the Monte Carlo methods are more time consuming but could have higher accuracy. For applications in tunnel fire safety, the discrete ordinates and the finite volume method are recommended to reduce the computation cost.

17.3.5.3 Heat Conduction

The general three-dimensional heat conduction equation for an anisotropic medium without an internal energy source can be expressed as:

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x_i}(k_{ij} \frac{\partial T_s}{\partial x_j}) \; i, j = 1, 2, 3 \tag{17.70}$$

where k is the thermal conductivity (kW/(m K)) and T_s is the temperature inside a solid (K). Subscript s indicates solid, i and j correspond to different axis, for example, x axis (1), y axis (2) or z axis (3). Note that for an anisotropic medium, such as wood, the conductivity varies with the direction.

Generally the medium is isotropic, such as the tunnel walls. Therefore, the above equation can be simplified into:

$$\rho_s c_s \frac{\partial T_s}{\partial t} = k_s (\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} + \frac{\partial^2 T_s}{\partial z^2}) \tag{17.71}$$

with boundary condition at the wall, for example, x = 0:

$$-k_{s,x} \frac{\partial T_s}{\partial x}\Big|_{x=0} = \dot{q}''_{w,net} \tag{17.72}$$

The net heat flux at the wall accounts for both radiation and convective heat transfer. In most cases, the equation can be simplified into a one-dimensional problem with sufficient accuracy. For example, the tunnel wall can be assumed to be an infinite plate. This governing equation is an energy diffusion equation which can be easily solved.

17.4 Recommendations for CFD Users

17.4.1 Computation Domain and Boundary Conditions

A tunnel is usually a very long space. Tunnel height and width are very small in relation to the tunnel length. Simulation of the whole tunnel may be impossible but is also not necessary in practice. While doing CFD simulations, an appropriate computation domain needs to be determined together with appropriate boundary conditions.

The computational domain should consist of the fire section and a certain length of tunnel section where the boundary conditions can be appropriately set without inducing large errors.

For a tunnel where longitudinal ventilation is used to prevent backlayering, a limited length including the fire section is enough. A velocity or volume flow rate or mass flow rate boundary can be used at the upstream tunnel inlet, and pressure or mass flow boundary can be used for the downstream tunnel outlet. It is best if the upstream section is long enough to simulate the whole backlayering. In this scenario, the reason why the downstream outlet can be considered as a pressure boundary is that at a certain distance downstream of the fire, the vertical pressure gradient is small and close to a fixed pressure plane, that is, the smoke is not well stratified. By setting the outlet as a pressure boundary, small errors will be induced for the field close to the exit. Therefore, the simulation results in this region are not credible, which should be considered in determination of computation domain. From this point of view, the mass flow rate is a better boundary condition for the outlet of the domain, although, convergence problems could emerge due to the accumulation of computation errors.

For a metro station or a rescue station in a long tunnel, the ventilation system may have many vents and thus many boundary conditions need to be determined. Further, the cross section is much larger than a single tunnel which suggests that a shorter length has to be used while choosing the computation domain. In this scenario, the boundary conditions of the computation domain have to be considered appropriately. Note that the ventilation system works as a system, and it is generally unreasonable to set the boundaries as ambient. The general solution is to obtain the time dependent boundary conditions by simulating the fire ventilation system using a one-dimensional simulation. For a vent where only fresh air goes in or out, velocity, volume or mass flow rate can be used. For each vent where hot gases may flow into, a volume flow rate boundary should normally be used rather than mass flow rate, for example, a fan vent could be simulated using a volume flow rate boundary or a fan curve. Another solution could be to use pressure boundaries if appropriate pressure values can be estimated based on a one dimensional simulation.

17.4.2 Fire Source

Modeling of fire development in vehicles is a difficult task which should be avoided in any case where it is not necessary. Generally for an engineering application, a typical or worst scenario is firstly determined and then the design fire is proposed

for the specific scenario. The design fire proposed is used as input to the CFD modeling of tunnel fires. There are different methods developed for modeling fires, for example, combustion models and volumetric heat source method. The volumetric heat source method only simulates the heat output and ignores the combustion process and combustion products. Therefore, radiation and convection heat transfer which is of greatest importance in large tunnel fires cannot be reasonably modeled. In the following, only the combustion models are of interest and discussed.

The chemical formula for the fuel generally needs to be determined. A fire could involve different types of fuels. In these cases, the combined chemical formula for the fuels can be obtained by accounting for the fraction of each fuel type. In the gas phase combustion, one step reaction is mostly assumed although the combustion occurs through a large number of reactions.

Some key parameters for the fuel also need to be known, that is, heat of combustion, soot yield, carbon monoxide yield. Heat of combustion, that is, the amount of heat produced per kg of the fuel, affects the production of combustion products. The soot yield, that is, the amount of soot produced per kg of the fuel, is required for modeling of radiation and visibility. Similar to the soot yield, the CO yield represents the amount of CO produced per kg of the fuel and is required for estimation of tenability. For CFD modeling related to toxicity, the toxic gas production also needs to be accounted for in the fire source in a similar way. The heat of combustion and the yields of soot, CO, and toxic gases can be obtained from small-scale laboratory tests of similar combustion conditions. Note that the yields of soot and combustion products depend on the combustion conditions, and they could be much higher in underventilated enclosures at the stage of fully developed fires. More information on combustion products in under-ventilated fires can be found in Chap. 7. Generally the fire in a tunnel is well ventilated and data obtained from lab tests could be directly used as input.

17.4.3 Grid Size

Grid cell size is a key issue related to both computation time cost and accuracy. For fire modeling, the fire region attracts our special attention. Note that the flame properties are directly related to the fire characteristic diameter, which can be expressed as follows [26]:

$$\left[D^* = \left(\frac{\dot{Q}}{\rho_o c_p T_o \sqrt{g}} \right)^{2/5} \right] \tag{17.73}$$

where $\dot{Q}$ is HRR (kW) and D^* is the fire characteristic diameter (m). Note that the characteristic diameter D^* is directly related to the HRR. Li et al.'s work concluded that a cell size of $0.075D^*$ is a reasonable value for simulation of tunnel fires [27].

Note that a smaller fire corresponds to a smaller cell size based on the above analysis. In a model-scale fire, the grid size is much smaller than that in full scale. For a tunnel with a height of H, Eq. (1) can be transformed into:

$$\frac{D^*}{H} = \left(\frac{\dot{Q}}{\rho_0 c_p T_o g^{1/2} H^{5/2}}\right)^{2/5} = Q^{*2/5} \tag{17.74}$$

where H is the tunnel height, regarded as the characteristic length here.

This means that at the same dimensionless HRR (Q^*), the fire characteristic diameter is directly related to the tunnel height, that is, the reasonable mesh size is proportional to the tunnel height. This means that the ratio of reasonable mesh sizes between model- and full-scale equals the scale ratio. In other words, the mesh numbers required for model- and full-scale is about the same. Note that this conclusion is deduced based on a similar flow mode and the same dimensionless HRR.

Another requirement for cell size results from wall stress and related heat transfer. For laminar flows, the first grid cell near wall needs to fall into the viscous layer, that is, y^+ is less than 1 or slightly higher but not higher than 11.63. For turbulent flows, the first grid cell requires to fall into the log layer, that is, $11.63 < y^+ < 500$. This generally affects not only the flow field but also the temperature field near the wall.

17.4.4 Verification of Modeling

Due to the complexity of CFD modeling itself and the variety of application fields, verification of modeling is a necessity, especially for modeling with any new application. Either data from full-scale tests or model-scale tests related to the same phenomenon can be used for verification, based on which the general uncertainty of CFD modeling can be obtained for the specific scenario.

17.5 Limitations of CFD Modeling

The current state-of-the-art of CFD modeling technique has many limitations.

The key limitation for fire modeling is the inability to fully model pyrolysis. Firstly, the fuels normally have complicated geometry and the thickness could be incompatible with the grid size, which suggests that the fuel and the fluid field are at different scales. Secondly, the pyrolysis is such a complicated phenomenon that the present models seldom succeed in pyrolysis modeling even for a simple sample test. The state-of-the-art pyrolysis models lack credibility and should only be used for research purpose at present.

Modeling of combustion requires very fine meshes in order to simulate a large number of flamelets. However, to reduce the computation cost, quite coarse grids

and infinite rate mixture fraction combustion model are normally used. Further, the flammability limit is not well established for the coarse girds. The approximate combustion model cannot model the combustion products.

The limitation of pyrolysis modeling directly results in the limitation for modeling of fire suppression, given that surface cooling is the key mechanism of suppression of tunnel fires in most cases. Another reason for the limitation in modeling of fire suppression is also that the extinction criteria or the flammability limit under fire suppression are not well established.

Radiation is one key mechanism of heat transfer especially in the vicinity of a large tunnel fire. However, the accuracy of modeling of flame radiation strongly depends on the accuracy of modeling of flames. Modeling of radiation from smoke depends on the yields of soot and other combustion products which are obtained either from lab tests or estimation of the typical fuel.

Convection heat transfer is in reality the heat conduction between a surface and its neighboring gas. The direct solution of convection heat transfer is only possible using DNS with very fine grids. For RANS and LES, the process of convection heat transfer has to be modeled by semi-empirical equations which could result in large errors in some cases. Especially for modeling of tunnel fires, the walls could be very rough and its effect on heat transfer may be overlooked, for example, in FDS [1].

CFD modeling strongly depends on the performance of computer hardware which is clearly a bottleneck. Recently, parallel processing is widely used in CFD modeling as a novel technology to reduce the computation time. However, this reduces the accuracy of CFD modeling, and could easily cause stability problems. Therefore, caution should be exercised in its application.

These limitations need to be kept in mind, together with the uncertainty obtained from verification of modeling in the specific application field.

17.6 Summary

CFD modeling is a powerful tool to be used in engineering applications. The CFD users are required to not only efficiently use CFD tools, but also to understand the embedded mechanisms and limitations of the CFD modeling used. At present, CFD modeling is mainly used to simulate smoke movement arising from a design fire in order to investigate the performance of a ventilation system on smoke control in a tunnel fire, and to simulate the fire environment to obtain the available evacuation time. It should be kept in mind that modeling of pyrolysis of fuels and fire suppression is still a difficult challenge at present.

Although, there have been many general CFD tools available, CFD tools specifically developed for use in fire modeling are recommended to be used in tunnel fire safety design. Due to the complexity of CFD modeling itself and the variety of application fields, validation of modeling is always required. The computation domain needs to be chosen appropriately together with the boundary conditions and the cell sizes.

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