CHAPTER 10

CFD fire simulation and its recent development

Z. Yan
Department of Building Science, Lund University, Sweden.

Abstract

This chapter presents an outline on computational fluid dynamics (CFD) fire simulations within the framework of Reynolds averaged Navier–Stokes (RANS), large eddy simulation (LES), and direct numerical simulation (DNS). First the general simulation concepts regarding RANS, LES, and DNS are briefly discussed with emphasis on the major theoretical difference between these three simulation concepts. This is followed by discussions on modeling of different essential sub-processes in fires. These essential sub-processes include turbulence, turbulent combustion, thermal radiation, soot formation, heat transfer inside solid, and pyrolysis of combustible solid fuel, etc. Within the discussion of sub-process modeling, some recent developments in sub-process modeling based on the author’s research are presented. Besides the discussion on the simulation of conventional fires, this chapter also presents techniques and some interesting recent developments on CFD simulation of spontaneous ignition in porous fuel storage.

1 Introduction

Computational fluid dynamics (CFD) simulation plays an important role in fire research. It provides a new efficient, reliable, and economic path for fire research and has become an essential fire research tool. Before the advent of CFD simulation, fire study was limited to experimental investigation and empirical correlation. Due to its high expense and practical difficulty, experimental data is usually very limited, if not unavailable. With the limited experimental data as validation base, a properly validated CFD simulation tool can provide much more information and thus extensively extrapolate the limited experimental data. In many cases, CFD simulation can also be used as pre-investigation of a to-be-performed experimental test and provide guidance for experiment. With the wide adoption of performance-based fire safety design, CFD simulation is becoming a routine practice for obtaining necessary fire design information. With new development in modeling techniques, fast increase of computing power, and quick drop of hardware price, it is expected for CFD simulation to continuously gain popularity in the fire community.

This chapter attempts to provide an outline on CFD simulation techniques for both conventional fires and spontaneous ignition in porous fuel storage.
2 CFD simulation of conventional fire

Figure 1 gives a simple illustration of a conventional fire. For CFD simulation of conventional fires, in most cases, turbulent combustion in gas phase, processes in bulk solid phases, and phase interaction need to be simultaneously taken into account. The turbulent combustion in gas phase is extremely complex. The processes in bulk solid may in general include the highly complicated internal heat, mass, and momentum transfer and chemical reaction. The interaction between gas and bulk solid concerns heat, mass, and momentum exchange.

2.1 Gas phase simulation

The gas phase process in the conventional fire considered in this chapter is in essence an unwanted turbulent combustion. The simulation of turbulent combustion in a conventional fire can in principle be carried out using the Reynolds averaged Navier–Stokes (RANS), large eddy simulation (LES), and direct numerical simulation (DNS) concepts.

2.1.1 Some basics of turbulence and turbulent combustion

Before we discuss RANS, LES, and DNS of gas phase turbulent combustion, it is necessary to present some very important basic physics of turbulence and turbulent combustion.

Turbulence remains one of the most challenging topics nowadays. It can be considered as a deterministic random hydrodynamic system. It is deterministic in a sense that for a unique set of initial and boundary conditions, the system is believed to hold a unique solution. It is random in a sense that when the Reynolds number of the flow is sufficiently high, the system becomes unstable. The flow solution in this case turns out to be very sensitive to external disturbances including the initial and boundary conditions.

Although it is very difficult to give an exact definition of turbulence, its general characteristic features can be identified [1]. The irregularity is one of the most important features of turbulence.
which is in contrast to the regularity of laminar flow. The random motion of turbulence enhances the mixing process drastically and turbulence is thus diffusive. Turbulence comes from the instability of the viscous flow at high Reynolds number, which results from the interaction between the viscous and non-linear inertial terms of the Navier–Stokes equations. The interaction is very complex and makes it a prohibitive task to fully analyze the flow instability. Turbulence holds a continuous spectrum of scales ranging from integral scales to Kolmogorov scales. It obtains its kinetic energy from the mean flow through shear and buoyancy production. The large eddies which have dimensions comparable to those of the mean flow contain most of the energy and thus are the energy containing eddies. The kinetic energy will largely be transferred to smaller eddies when the smaller eddies are stretched by the larger eddies. Most of the turbulence kinetic energy will be dissipated at the smallest eddies. Therefore, turbulence is always dissipative. In the inertial range of eddies if we ignore the small dissipation the energy received from the larger eddies is equally transferred to the smaller eddies. This gives the picture of the turbulence kinetic energy cascade. The rotational nature of turbulence and the turbulence maintaining mechanism of vortex stretching bring turbulence to a three-dimensional space, because vortex stretching does not exist in a two-dimensional space. The dissipative character of turbulence is closely related to rotational motions. The rotation of the flow favors the creation of many regions of large gradients and thus enhances the dissipation.

Turbulence has a wide range of scales. The turbulence eddy size can range from the integral length scale to the Kolmogorov length scale. The integral length scale \(l\) is comparable to a physical dimension of the problem under consideration. The Kolmogorov length scale is the length scale of the smallest eddies in a turbulent flow. According to Kolmogorov’s theory [1–3], the size of smallest eddies can be estimated as \(\eta = (\nu^3/\epsilon)^{1/4}\), where \(\nu\) is the kinematic viscosity and \(\epsilon\) is the turbulence kinetic energy dissipation rate which can be estimated as \(\epsilon = (u'^3)/l(u') = (u'^3)/l\). The Kolmogorov length scale can be as small as 0.1 mm. Turbulence time scales also vary from the integral time scale of the large eddies to the Kolmogorov time scale of the smallest eddies. The integral time scale is of the order \(l/u'\), where \(u'\) is the rms value of velocity fluctuations. The Kolmogorov time scale can be estimated as \(\tau = (\nu/\epsilon)^{1/2}\). The ratio of the integral time scale to the Kolmogorov time scale is the square root of the Reynolds number which is usually quite large.

In turbulent reacting flow, chemical reaction is another very complicated factor. Even for simple fuels, the chemistry may comprise thousands of reactions. In the reactions, the time scale can also vary by several orders of magnitude, going from the fast heat release reactions to the slow pollution formation reactions such as the NO\(_x\) and soot formation.

Meanwhile there is a strong interaction between combustion and turbulence. Both of them have dual effects on each other. The heat released by combustion will cause the thermal expansion of the fluid mixture, thus driving a flow. The viscous flow may loose its stability when the Reynolds number of the flow is sufficiently high and the transition from laminar flow to turbulent flow may happen. On the other hand the reduction of the fluid density has a damping effect on vorticity, diminishing turbulence. Meanwhile, turbulence also has dual effects on combustion. In a diffusion flame, the fuel and oxidant need to be mixed at the molecular level first before the reaction can happen. In a premixed flame, the flame propagation depends on the heat conduction and the diffusion of radicals from the burned region to the unburned region. Many chemical reactions have much smaller time scales than the physical mixing process. Thus the mixing is often crucial for combustion and the turbulent combustion often turns out to be mixing controlled in a general sense. As a result, the turbulence, which can enhance mixing, may intensify combustion, in both diffusion and premixed flames. However, strong turbulence may also affect the flame structure and increase the flame heat loss rate to such an extent that the flame may be extinguished by the high strain rate [4–6].
Depending on the relation between flow and reaction scales, turbulent combustion can fall into several distinguished regimes. The ratios of the corresponding flow scales and reaction scales define several non-dimensional numbers, including the Reynolds number, Damköhler number, and Karlovitz number. These numbers have their clear physical interpretation and thus give some indication on the status of the combustion. Borghi’s diagram gives a good conceptual description on this point for a premixed flame (see [6−8] for details).

Accurate modeling of turbulent combustion requires a proper consideration of all the important physics and chemistry. The physical aspects briefly discussed above give some important clues for the modeling strategy and possible simplifications. In turbulence modeling, the spectrum of the turbulence scales explains why conventional turbulence modeling cannot be universally applicable. The length and time scales of the large eddies are comparable to those of the mean flow. As a result, turbulence is a property of the flow. Any conventional turbulence model, which is tuned for certain types of flow, may fail in other situations. In LES, since the modeled small eddies do not have a strong direct interaction with the mean flow, the LES modeling can be expected to be more universal.

Concerning the combustion modeling, when the time scale of the chemistry is much smaller than that of mixing, the combustion is mixing controlled and one may reasonably assume that combustion happens once the fuel and oxidant are mixed. The mixing control assumption allows the combustion analysis to be significantly simplified. This is the starting point of Magnussen’s eddy dissipation concept (EDC) combustion model [9, 10] which will be discussed later. The fast chemistry assumption is also one of the key points in the development of the flamelet combustion model [11−17], where the turbulent flame is considered to be an ensemble of wrinkled laminar flamelets which have a well-defined structure.

2.1.2 CFD simulation of turbulent combustion in a conventional fire

CFD simulation of fires corresponds to numerically solving a set of governing equations which describe the physics of interest.

For the gas phase turbulent combustion in a conventional fire, the governing equations, comprising continuity, momentum, energy, and species equations, are:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] + \rho a_{gi}
\]

\[
= \frac{\partial p^*}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] + (\rho - \rho_\infty) a_{gi}
\]

\[
\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u_i h)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial h}{\partial x_j} \right) + S_h
\]

\[
\frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho u_i Y_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial Y_i}{\partial x_j} \right) + R_i
\]

where \( p^* = p - \rho_\infty + \rho_\infty a_{gi} x_i \) is the pressure minus its hydrostatic value, \( x_i \) is the space coordinate vector, \( t \) is the time, \( \rho \) is the density, \( u_i \) is the velocity vector, \( h \) is the enthalpy, \( \mu \) is the dynamic viscosity, \( S_c \) is the Schmidt number, \( Pr \) is the Prandtl number, \( Y_i \) is the mass fraction for chemical
species \(i\), \(\delta_{ij}\) is the Kronecker delta tensor, \(a_{gi}\) is the gravity acceleration vector, \(R_i\) is the reaction rate, \(S_h\) is the energy source term resulting from the radiation, and

\[
h = \sum Y_i h_i = \sum Y_i \left( h_{0,i} + \int \frac{T}{\alpha} c_p dT \right)
\]

in which \(h_{0,i}\) is the heat of formation of species \(i\) at temperature \(T_0\).

The radiation equation and the thermal state relations provide the necessary auxiliary equations.

With this set of established mathematical equations, the task left is to build up proper initial and boundary conditions for a concerned particular case and using numerical methods to find out the solution.

While pursuing a numerical solution of the above governing equations, one has to deal with space and time discretization. This raises the resolution issue. This resolution issue is critically important for CFD computations. Numerical resolution must be very carefully examined with regard to the physical scales described by the equations to be solved. The principle which has to be followed for a numerical computation of a turbulent reacting flow is that the adopted numerical resolution must be fine enough to resolve all the concerned physical scales described by the governing equations to be solved. This principle will be explained in detail in the following sections. Any numerical computation performed without following this principle loses its fundamental base and thus does not really have much physical meaning, even though the computation may still be able to produce colorful pictures. In CFD, due to different reasons and variable concerns, the physical scales that need to be resolved may vary from case to case. Basically three different simulation concepts can be constructed depending on what physical scales are to be resolved. These three simulation concepts are the well-known RANS, LES, and DNS concepts which will be discussed below.

### 2.1.2.1 Direct numerical simulation

In DNS, the Navier–Stokes equations are solved in original form without any pre-treatment. With regard to turbulence, the physical scales described in the Navier–Stokes equations in original form cover the whole turbulence spectrum, ranging from the integral scales to Komogorov scales. Each individual eddy in a turbulent flow can be characteristically seen as a ‘kingdom’. Therefore, in order to implement DNS, one has to resolve the smallest scales properly, in both space and time coordinates.

As discussed before, Kolmogorov length scale can be estimated as \(\eta = (\nu^3/\epsilon)^{1/4}\) and is related to the integral length scale as \(\eta l = Re^{-3/4}\), where \(Re\) is the Reynolds number \(Re = u' l / \nu\) which is usually quite large. Similarly, one can easily show that the ratio of the integral velocity scale to the Kolmogorov velocity scale \(v\) is the one-fourth power of the Reynolds number, and the ratio of the integral time scale to the Kolmogorov time scale is the square root of the Reynolds number. Therefore, in a three-dimensional turbulent flow computation, with an increase in Reynolds number, the grid size decreases according to \(Re^{-3/4}\) and consequently the grid number increases according to \((Re^{3/4})^3 = Re^{9/4}\). In a DNS computation, an explicit scheme is normally adopted and the time step size is numerically limited by the Courant–Friedrichs–Levy (CFL) stability condition \(u \Delta t / \Delta l \leq 1\), where \(u\) is flow velocity, \(\Delta t\) is the allowed time step size and, \(\Delta l\) is the grid size. This indicates \(\Delta t \leq \Delta l / u\). Meanwhile, approximately, \(u = u'\). For the smallest eddies, we also have \(\tau = \eta v = \eta u' (Re^{-1/4}) = \eta (Re^{1/4}) u'\). Since the computational grid needs to resolve the smallest eddies one can write \(\Delta l = \eta\). Therefore, \(\Delta t < \tau\). This indicates that with explicit time marching the time step size limited by the CFL condition must be small enough to resolve the Kolmogorov
time scale. Consequently, assuming the CPU time for solving algebraic equations is linearly proportional to the number of unknowns, the computational effort can be indicated by the product of grid number and the number of time steps which is given by \( t/\Delta t = (l/u)/(\Delta l/u) \). Based on the above discussion, the computation effort can be shown to be proportional to \( Re^{9/4}(l/u)(\Delta l/u) = Re^{9/4}/l = Re^{9/4}/\eta = Re^{3/2}Re = Re^{3} \). As a result, the resolution required in DNS turns out to be very computer resource demanding and thus creates resolution problem for DNS. At present, even with massive parallel computers, DNS is only possible for some simple flows.

While doing DNS, the resolution must be fine enough to capture the smallest eddies. However, this is not yet enough. There is also some requirement on the employed numerical scheme. A high order numerical scheme is needed to minimize numerical diffusion which otherwise may overpower the physical diffusion associated with the fluid. It should be noted that the viscosity for normal gas such as air has a very small value and thus can easily be distorted if the numerical scheme is not adequate. Furthermore, a turbulent flow system is unstable. The flow solution is very sensitive to external disturbances including the initial and boundary conditions. Therefore, the treatment of initial and boundary conditions must be very carefully examined.

For DNS of fires, consideration must be given to the additional sub-processes such as chemical reaction. In fires, both premixed and non-premixed flame may exist. In chemical reactions, the time scale can also vary by several orders of magnitude going from the fast heat release reactions to the slow pollution formation reactions such as soot formation. The time scales of all the relevant chemical reactions must be properly resolved. Meanwhile, spatial resolution consideration also needs to be given to flame thickness which can be very small. Strictly speaking, to really implement DNS for fires, the detailed chemistry must also be known and included. This brings extra difficulty. Currently, it is prohibitive to do any DNS on practical fires.

### 2.1.2.2 Reynolds averaged Navier–Stokes

To overcome the resolution problem associated with DNS, one has to relax the to-be-resolved physical scales. The to-be-resolved physical scales are associated with the governing equations. To have the needed relaxation, one way is to do some pre-treatment on the governing equations. Perhaps we can call a simulation concept within this framework a relaxed simulation. In this sense, both RANS and LES can be seen as relaxed simulation methods, although the pre-treatments on the governing equations in RANS and LES are different. Meanwhile, this also provides flexibility with the numerical schemes and initial and boundary conditions. However, one should note that there is one requirement for the pre-treatment. That is the relaxed solution should be able to deliver the intended information.

RANS is one commonly used cheap relaxation method where the pre-treatment applied on the original instantaneous equations corresponds to statistical averaging. This pre-treatment is widely adopted in engineering computations because the most concerned is the mean flow property in many practical engineering applications. Since the instantaneous governing equations are statistically averaged for solution, only the relatively smooth mean field needs to be resolved properly. Therefore, the to-be-resolved physical scales are much larger than those found in DNS. In this way, the resolution issue can be very much relaxed so that simulation of practical complex turbulent flows can be handled using currently available computers. However, it should be noticed that the statistical averaging pre-treatment does not really help wipe out the problem associated with DNS. Instead, this pre-treatment is a kind of problem shift mechanism. The resolution problem is removed at the price of a closure problem. By doing statistical averaging, extra terms representing the contributions of fluctuations to the averaged field show up in the pre-treated governing equations. Models must be constructed to represent these contributions.
In conventional fires where flow velocity is of the order of several meters per second (Mach number \(< 1.0\)), with bulk viscosity and Dufour and Soret effects ignored, the set of Favre-averaged governing equations for fire simulation can be written as:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i)}{\partial x_i} = 0 \quad (6)$$

$$\frac{\partial (\bar{\rho} \bar{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_j \bar{u}_i)}{\partial x_j} = \frac{-\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} - \bar{p} \bar{u}_i \bar{u}_j \right] + \rho \bar{a}_{ki} \quad (7)$$

$$\frac{\partial (\bar{\rho} \dot{h})}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \dot{h})}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{P_r} \frac{\partial \dot{h}}{\partial x_j} - \bar{p} \bar{u}_i \bar{u}_j \right) + \bar{S}_h \quad (8)$$

$$\frac{\partial (\bar{\rho} \bar{Y}_i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i \bar{Y}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{S_c} \frac{\partial \bar{Y}_i}{\partial x_j} - \bar{p} \bar{u}_i \bar{Y}_j \right) + \bar{R}_i \quad (9)$$

where the over bar represents Reynolds averaging, the tilde represents Favre averaging, and the double prime represents the fluctuation from Favre averaging.

The mean enthalpy source term \(\bar{S}_h\), mean reaction rate \(\bar{R}_c\), and the second moments such as \(-\bar{p} \bar{u}_i \bar{u}_j \) and \(-\bar{p} \bar{u}_i \bar{u}_j \bar{h} \) arise from the averaging operation of the governing equations. They need to be modeled and will be discussed in modeling section.

Figure 2 gives a typical temperature profile from a RANS simulation of a buoyant flame. Obviously, the presented plot represents an averaged profile.

The main advantage of RANS is its simplicity and computational efficiency. However, because the energy containing large eddy scales within the turbulence spectrum are comparable to the scales of the mean flow, turbulence is a property of the flow. As a result, the constructed turbulence models in RANS can never be universal. Any conventional turbulence model, which is tuned for certain types of flow, may fail for others.

### 2.1.2.3 Large eddy simulation

LES is another relaxed simulation method, which lies between DNS and RANS. In LES, the pre-treatment involves spatial filtering. This filtering provides a scale separation where the turbulence scales are separated into resolved scales and unresolved scales. In LES, eddies down to the inertial sub-range are properly resolved. The contribution of smaller eddies is modeled using sub-grid models. In a turbulent flow, large energy containing eddies are directly subject to geometry and boundary conditions. These large eddies are highly flow-dependent and play a major role in transport. They are resolved in LES. The remaining small unresolved eddies are not tuned in the same range of frequency of the mean flow. Therefore, sub-grid modeling of contribution from small eddies can be expected to be relatively more universal than the turbulence modeling in RANS. Since the resolution goes down to the inertial
sub-range, the needed resolution can be rather fine. Due to the adopted fine spatial and temporal resolutions, LES also reveals more detailed flow dynamics and structure. However, these advantages come at a price. Because of the adopted fine resolution, LES is much more computer resource demanding. Meanwhile, compared to the RANS equations, the filtered transport equations in LES are much less dissipative and consequently the solution of the filtered equations in LES is usually much more sensitive to the specified boundary and initial conditions. Both the initial and boundary conditions may have a significant effect on the simulation. For example, a numerical study in [18] reported a strong effect of initial conditions on LESs of a thermal plume. Unfortunately, a proper specification of initial and boundary conditions for LES remains a difficult task. During past years, much research has been done to find out proper specifications of boundary conditions for different boundaries in flow computations [19–22].

It should be emphasized that the resolution must be enough to resolve down to the inertial sub-range in an LES computation. As a very rough guidance, this required resolution can be estimated by the Taylor microscale which is defined as $\lambda = \sqrt{\frac{u^2}{\nu \partial u / \partial x}}$. In isotropic turbulence, the Taylor microscale is related to dissipation rate as $\varepsilon = 15 \nu^3 / \lambda^2$, where $\nu$ is the kinematic viscosity and $u$ is the rms value of velocity fluctuations. Without proper resolution, a computation cannot be accepted as a LES computation and does not have a scientific basis from a LES point of view. Before presenting a LES computation, the numerical resolution needs to be examined to show it is adequate. This examination can be made by analyzing the spectrum of the turbulence kinetic energy to make sure that eddies down to the inertial sub-range are properly resolved. Figure 3 shows a typical turbulence energy spectrum at a location on the center line in a three-dimensional computation of a buoyant plume [23]. As can be seen in this computation, with some substantial inertial sub-range predicted, the theoretical Kolmogorov $-5/3$ decay was fairly well captured in the computation. This indicates that the spatial resolution used in the computation is adequate.

Large eddy simulation of conventional fires is based on the solution of a set of density weighted spatially filtered conservation equations, comprising continuity, momentum, energy, and species equations. Turbulence and turbulent combustion sub-grid scale (SGS) models overcome the

Figure 2: A typical temperature profile from a RANS simulation of a buoyant flame.
closure difficulty resulting from filtering the partial differential equations. The radiation equation and the thermal state relations provide the necessary auxiliary equations.

Assuming that the error arising from the commutation of filtering operation and differentiation for a used non-uniform grid is absorbed in the SGS models, the filtered equations have a form that is similar to those in RANS and can be written as:

\[ \frac{\partial \tilde{r}}{\partial t} + \frac{\partial (\tilde{r} \tilde{u}_i)}{\partial x_i} = 0 \]  

(10)

\[ \frac{\partial (\tilde{r} \tilde{u}_i)}{\partial t} + \frac{\partial (\tilde{r} \tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} + \tau_{ij} \right] + \tilde{p} \tilde{u}_i \]  

(11)

\[ \frac{\partial (\tilde{h})}{\partial t} + \frac{\partial (\tilde{h} \tilde{u}_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr} \frac{\partial \tilde{h}}{\partial x_j} + q_{j,h} \right) + S_h \]  

(12)

\[ \frac{\partial (\tilde{Y}_j)}{\partial t} + \frac{\partial (\tilde{Y}_j \tilde{u}_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc} \frac{\partial \tilde{Y}_j}{\partial x_j} + q_{j,Y} \right) + \tilde{K}_j \]  

(13)

where the over bar and the tilde represent spatial filtering and Favre spatial filtering, respectively. In the above equations, the filtered enthalpy source term \( S_h \), the filtered reaction rate \( \tilde{R}_r \), the SGS stress \( \tau_{ij} \), and the SGS scalar fluxes including \( q_{j,h} \) and \( q_{j,Y} \) need to be modeled and will be discussed in the modeling section.

Figure 3: Turbulence energy spectrum at a location of the center line in a simulated thermal plume.
The spatial filtering operation on a variable $\varphi$ is given by

$$\bar{\varphi}(\vec{r}, t) = \int_{V} G(|\vec{r} - \vec{r}'|) \varphi(\vec{r}') d\vec{r}'$$

(14)

and the Favre spatial filtering operation is defined as

$$\tilde{\varphi}(\vec{r}, t) = \int_{V} G(|\vec{r} - \vec{r}'|) \varphi(\vec{r}') \rho(\vec{r}') d\vec{r}' / \int_{V} G(|\vec{r} - \vec{r}'|) \rho(\vec{r}') d\vec{r}' = \bar{\rho} \bar{\varphi} / \bar{\rho}$$

(15)

where $\vec{r}$ and $\vec{r}'$ are space vectors, $V$ is the volume of filtering, and $G(|\vec{r} - \vec{r}'|)$ is a filter function which must satisfy the normalization condition $\int_{V} G(|\vec{r} - \vec{r}'|) d\vec{r}' = 1$.

The SGS stress tensor $\tau_{ij}$ includes the Leonard, cross and Reynolds SGS stresses which can be written as $-\tilde{\rho} \tilde{u}_i \tilde{u}_j + \tilde{p} \delta_{ij} - \tilde{\rho} \tilde{u}_i \tilde{u}_j$ and $-\tilde{p} \tilde{u}_i \tilde{u}_j$ and $-\tilde{p} \tilde{u}_i \tilde{u}_j$. Similarly, the SGS flux $q_{i,\varphi}$ for a general scalar $\varphi$ has three components $-\tilde{\rho} \tilde{u}_j \tilde{\varphi} + \tilde{p} \delta_{ij} \tilde{\varphi} - \tilde{\rho} \tilde{u}_j \tilde{\varphi}$ and $-\tilde{p} \tilde{u}_j \tilde{\varphi}$.

In LES, instantaneous distributions are computed like the one shown in Fig. 4, which may look more realistic than the profile obtained in RANS according to one’s real life impression. However, for practical engineering application, in many cases, people need to know the mean distributions (statistics). In LES, the statistics are obtained by averaging a large number of instantaneous profiles over a sufficient time period. The higher the order of the desired statistics, the longer the time period required for averaging. Some discussions on averaging and the averaging time can be found in [23].

2.1.3 Modeling of gas phase sub-processes in a conventional fire

When pursuing the simulation of a conventional fire using computers, a set of mathematical equations are numerically solved. In the governing and the necessary auxiliary equations, for certain terms

![Instantaneous temperature profile](Figure 4: A typical instantaneous temperature profile from a LES of a buoyant diffusion flame.)
and/or variables, due to limits in scientific knowledge, there may be a lack of proper fundamental description. In this case, models are needed to provide approximations for those unknowns which may either already exist in the original equations constructed from physical laws or come from the pre-treatment of the original equations. The models can be constructed in the form of mathematical formula(s) and/or through a set of additional model differential equations.

For CFD fire simulations, depending on which simulation concept is used, the gas phase sub-process modeling mainly covers turbulence, turbulent combustion, radiation, and soot formation.

2.1.3.1 Turbulence modeling

As was already discussed, modeling is explicitly needed for consideration of turbulence when the RANS or LES simulation concept is adopted. The main purpose of turbulence models is to provide modeling for the unknown terms arising from the pre-treatment of the Navier–Stokes equations. In DNS, the original instantaneous equations are solved, turbulence is fully accounted for in those equations and thus no explicit model should be used.

2.1.3.1.1 Turbulence model in RANS

The turbulence modeling closure problem in RANS can be addressed by constructing turbulence models, which are used to somehow feed back the contribution of fluctuations to the mean fields. Many different turbulence models, of varying complexities and applicabilities, have been proposed [24], such as the mixing length model, the $k$–$e$ model, the $k$–$\omega$ model, the algebraic stress model (ASM), and the Reynolds stress model (RSM). Consideration should be given to both applicability and simplicity when selecting a specific turbulence model for a given application. Due to the complexity, the closure is often constructed heavily based on dimensional arguments with the closure ‘constants’ (if there is any) derived from relatively well-defined flows. The lack of full physics prevents the closure to be universal. As a result, a model or closure, which is applicable to certain types of flow, may fail when applied to other types of flow.

The confidence of applying a turbulence model to a specific type of flow can only be obtained through extensive validation and testing. In particular, a turbulence model should be used with care when it is applied to a flow with a condition under which the closure assumption introduced in the model development can seriously be violated. When applying a turbulence model, for numerical reasons, the simplicity and numerical stability of the turbulence model is also highly concerned. Therefore, the choice of a turbulence model mainly depends on the simulation objectives and the compromise between accuracy and simplicity.

The standard $k$–$e$ model: The standard $k$–$e$ model is perhaps one of the most widely used models. Like all the other turbulence models it has its own serious defects such as limited applicability to flow of strong streamline curvature or strong rotation [24]. The defects of the standard $k$–$e$ model originate from the closure assumptions including the adopted Boussinesq assumption which assumes a linear relation between the Reynolds stress and the mean strain rate. The Boussinesq assumption may fail when the flow is subject to a sudden change of strain rate or a strong rotation. When scalar transport is involved, the simple gradient modeling procedure is normally adopted for the scalar fluxes within the framework of the standard $k$–$e$ model. This introduces additional defects and leaves space for improvement. However, the standard $k$–$e$ model has its important advantages that it is simple, numerically stable, and has been proved successful in many practical applications. Strategies are suggested to abandon the Boussinesq assumption, for example, by constructing a non-linear relation between Reynolds stress and the mean strain rate, solving algebraic Reynolds stress equations or differential Reynolds stress equations. However, all of these alternatives have their own deficiencies with respect to their complexities and modeling uncertainties. For example, in the RSM up to seven additional differential equations need to
be solved and the modeling of the pressure strain redistribution term is still a challenge. Therefore, the standard \( k - \varepsilon \) model remains attractive.

When applied to buoyant flows, the standard \( k - \varepsilon \) model needs to be modified to include the important buoyancy effect on turbulence and turbulent transport. In this buoyancy modified \( k - \varepsilon \) model, two turbulence quantity equations are solved

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho \bar{u}_i k)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu_t \frac{\partial k}{\partial x_j} \right) + \rho (P + G - \varepsilon) \tag{16}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \bar{u}_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu_t \frac{\partial \varepsilon}{\partial x_j} \right) + c_{\varepsilon} \rho \frac{\varepsilon^2}{k} (P + G)(1 + c_{\varepsilon} R_f') - c_{\varepsilon}^2 \rho \frac{\varepsilon^2}{k} \tag{17}
\]

where \( P = -\bar{u}_i^\prime \bar{u}_j^\prime \frac{\partial \bar{u}_j}{\partial x_i} \) and is modeled as \( P = \frac{\nu_t}{Re} \left( \frac{\bar{u}_i^\prime}{\bar{u}_j^\prime} \right) \frac{\partial \bar{u}_j}{\partial x_i} \), \( R_f' \) is the modified flux Richardson number \(-G/(G + P)\), \( G = -\beta \frac{\partial T}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_i} \| \bar{a}_g \| \) and is modeled as \( G = \beta \frac{\partial T}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_i} \). \( \beta \) is the thermal expansion coefficient \(-1/\kappa \) and \( \kappa \) is modeled as \( \kappa = 1.0 \) and \( \kappa = 0.7 \) for vertical and horizontal flows, respectively.

The solution of the partial differential equations for turbulence kinetic energy and its dissipation rate provides an estimate of the rms value of the velocity fluctuation, \( \bar{u}_i^\prime \), and a characteristic turbulence length scale, \( l \), as: \( u \sim \bar{u}_i^\prime \) and \( l \sim k^{1/3} \). With the dimensional arguments and an analogy to molecular mixing, they can be used to compute the eddy viscosity \( \mu_t \sim \rho u l \), which is used in the Boussinesq approximation to model the Reynolds stress tensor \(-\rho \bar{u}_i^\prime \bar{u}_j^\prime \). The Reynolds stress modeling reduces to \(-\rho \bar{u}_i^\prime \bar{u}_j^\prime = \mu_t \left( \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) \) when the divergence of averaged velocity field is ignored. This provides the closure for the averaged momentum equation. The turbulent scalar fluxes \(-\rho \bar{u}_i' Y_i'^\prime \) and \(-\rho \bar{u}_i'' h'' \) are modeled similarly by using the simple gradient modeling method with turbulent Prandtl/Schmidt numbers introduced.

Values of the various constants used in the model and the corresponding references are listed in Table 1.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_\mu )</td>
<td>0.09</td>
<td>13</td>
</tr>
<tr>
<td>( C_{1c} )</td>
<td>1.44</td>
<td>13</td>
</tr>
<tr>
<td>( C_{2c} )</td>
<td>1.92</td>
<td>13</td>
</tr>
<tr>
<td>( C_{3c} )</td>
<td>(a) 0.0</td>
<td>13</td>
</tr>
<tr>
<td>( \sigma_k )</td>
<td>1.0</td>
<td>13</td>
</tr>
<tr>
<td>( \sigma_\varepsilon )</td>
<td>1.3</td>
<td>13</td>
</tr>
<tr>
<td>( \sigma_T )</td>
<td>0.7</td>
<td>14</td>
</tr>
<tr>
<td>( \sigma_P )</td>
<td>0.7</td>
<td>14</td>
</tr>
<tr>
<td>( \sigma_g )</td>
<td>2.0</td>
<td>14</td>
</tr>
</tbody>
</table>

Note: (a) is for vertical flow and (b) is for horizontal flow.
An improved $k-e$ model: The modeling procedure in the above standard buoyancy-modified $k-e$ model is simple, but has been found inadequate for the modeling of buoyant turbulent flows. It cannot capture counter gradient diffusion and tends to significantly under-predict the spreading rate of vertical thermal plumes \[25, 26\] and over-predict the spreading rate of horizontal, stably-stratified flows \[27\]. Counter gradient diffusion is an important point which should be considered in the modeling of buoyancy driven turbulent flows. The heated gas has a low mass density, thus can be preferentially accelerated by pressure difference, and consequently may feature counter gradient diffusion \[28\]. The incorrect prediction of the spreading rates can bring serious deficiencies to the prediction of the important velocity and scalar profiles.

A modified $k-e$ two-equation turbulence model was developed in \[29\], to improve the consideration of buoyancy effects. This modified model was found to be stable, computationally economic and applicable to complex situations. It is capable of capturing counter gradient diffusion and well predicts the plume spreading rates and velocity and temperature profiles.

In this improved model, the generalized gradient diffusion hypothesis is adopted to replace the simple gradient diffusion for modeling of turbulent scalar fluxes. In particular, the $\overline{u''_i T''}$ term in the buoyancy production of turbulence kinetic energy $G = -\beta \overline{u''_i T''} a_{ij}$ is modeled using generalized gradient diffusion as

$$
\overline{u''_i T''} = -c_i \frac{k}{\varepsilon} \overline{u''_i u''_j} \frac{\partial \overline{T}}{\partial x_j}
$$

where $c_i = \frac{3}{2} c_m / \sigma_T$.

It was found in \[29\] that the generalized gradient diffusion modeling of $\overline{u''_i T''}$ provides a better representation of $G$.

To consider a direct effect of buoyancy on $\overline{u''_i u''_j}$ as indicated by the ASM formula, the turbulence kinetic energy shear production term $P$, which appears in both $k$ and $\varepsilon$ equations, is computed as

$$
P = (P)_{\text{std}} (1 - R_f)
$$

where $(P)_{\text{std}} = u_i \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial \overline{u_i}}{\partial x_j}$ is the turbulence kinetic energy shear production modeled in the standard buoyancy-modified $k-e$ model.

In consistency with modeling of the heat flux $\overline{u''_i T''}$, all the scalar fluxes such as $\overline{u''_j h''}$ and $\overline{u''_j Y_i}$ are modeled in a generalized gradient diffusion form.

All the empirical model constants keep their values from the standard $k-e$ model except for $c_{3e}$, which is directly related to buoyancy effect. In the standard buoyancy-modified $k-e$ model, different values of $c_{3e}$ were recommended \[30\], varying with flow conditions from about 0.0 to 1.0. In this improved model, a value of 0.6 is recommended for $c_{3e}$, largely based on numerical experiments.

When compared with the standard buoyancy-modified $k-e$ turbulence model, this model gives significantly improved numerical results as illustrated in Fig. 5.

2.1.3.1.2 Sub-grid scale turbulence model in LES In LES, the unknown sub-grid stress tensor and sub-grid scalar fluxes in the filtered momentum and scalar transport equations must be modeled in terms of the properties of the resolved scales so that the equation system can be closed. A good SGS model should be able to properly remove the turbulence kinetic energy from the resolved scales and account for backscatter of turbulence energy. Smagorinsky proposed the
first SGS model in 1963 [31]. Since then, many SGS models such as the similarity model [32] and the dynamic model [33, 34], have emerged. Although the Smagorinsky SGS model does not allow turbulence energy backscatter from small to large scales, it remains popular due to its simplicity and effectiveness. It has been used in many LESs. Considering its popularity, the Smagorinsky model is briefly presented below.

In the Smagorinsky SGS model, the SGS stress tensor is modeled by

$$\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = 2\mu_{sgs} \tilde{S}_{ij}$$

(20)

which is based on the eddy viscosity concept similar to that in RANS.

The strain rate tensor is given by

$$\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$

(21)

An approximation of the SGS eddy viscosity $\mu_{sgs}$ can be obtained by assuming local equilibrium of small eddies. The dissipation rate can be estimated by $\varepsilon = \frac{k_{sgs}}{\tau}$, where $k_{sgs}$ is the sub-grid kinetic energy and $\tau$ is the sub-grid time scale. The sub-grid time scale can be represented by $\tau = \Delta k_{sgs}^{0.5}$, where $\Delta$ is the filter width. Meanwhile, the SGS kinematic viscosity can be approximated as $\nu_{sgs} = k_{sgs}^{0.5} \Delta$. Therefore, we have $\nu_{sgs} = \varepsilon^{1.5} \Delta^{0.5}$. The production of SGS turbulence kinetic energy can be given by $P_K = \nu_{sgs} \left( 2 \tilde{S}_{ij} \tilde{S}_{ij} - \frac{1}{p} \frac{\partial \rho}{\partial t} \frac{1}{\tau_{ij}} \frac{\partial \tau_{ij}}{\partial x_i} \right)$. Finally, by assuming the equilibrium condition $\varepsilon = P_K$, after some simple mathematics, we have the buoyancy-modified Smagorinsky model where the SGS viscosity can be approximated as

$$\nu_{sgs} = C_s^2 \Delta^2 \left( 2 \tilde{S}_{ij} \tilde{S}_{ij} + P_B \right)^{0.5}$$

(22)

where $P_B$ is the buoyancy production term $-\frac{1}{p} \frac{\partial \rho}{\partial t} \frac{1}{\tau_{ij}} \frac{\partial \tau_{ij}}{\partial x_i} a_{ij}$ and $C_s$ is the case dependent Smagorinsky ‘constant’. The standard Smagorinsky model can be recovered from eqn (22) by simply excluding the buoyancy production term $P_B$. The case dependent Smagorinsky ‘constant’ $C_s$ usually has a value between 0.1 and 0.2.

Figure 5: Comparison of predicted and measured temperature and velocity profiles at 90 cm above a buoyant C3H6 diffusion flame [29] (©Elsevier Science Ltd, with permission).
The SGS turbulent scalar flux $q_{j,\varphi}$ for scalar $\varphi$ arising from the filtering of a scalar transport equation is modeled using a simple gradient transport hypothesis, as

$$q_{j,\varphi} = \frac{\mu_{sgs}}{\sigma_{\varphi}} \frac{\partial \varphi}{\partial x_j}$$  \hspace{1cm} (23)

where $\sigma_{\varphi}$ is the SGS turbulent Prandtl/Schmidt number for scalar $\varphi$.

2.1.3.2 Turbulent combustion models

Turbulent combustion models are adopted to cope with the closure problem created by pre-treating the non-linear reaction rates. There are different combustion models available. In this chapter, the discussion is limited to two basic strategies popularly employed for fire simulation. One is to solve the pre-treated transport equations of the non-conserved mass fractions with the pre-treated chemical reaction rates directly modeled. Another one is to solve the transport equation of a conserved scalar and then relate the concerned pre-treated non-conserved mass fractions to the conserved scalar using the laminar flamelet concept and a probability density function. They are briefly discussed below.

2.1.3.2.1 Eddy dissipation concept in RANS

The eddy dissipation concept proposed by Mognussen and Hjertager [9] is a popular representative method in RANS to model the mean reaction rate directly. It has gained its popularity since it is simple and widely applicable.

In a diffusion flame, the fuel and oxidant need to be mixed at the molecular level before a reaction can happen. In a premixed flame, the flame propagation is dependent on the mixing of hot products with the unburnt mixture and the diffusion of radicals. The chemical kinetics determines how the reaction will proceed in the mixture. Therefore, combustion depends on both mixing and chemical kinetics in general, but is essentially controlled by the slower of these two sequential processes, particularly when the slower process is much slower than the faster one. When the chemistry is much faster than the mixing, combustion turns out to be mixing-controlled. In this case, the mixing rate can well represent the combustion rate.

The mixing process in a turbulent flow is largely dependent on the property of the turbulence. In a turbulent flow, there exists a kinetic energy cascade, which was already discussed earlier. The turbulence kinetic energy is extracted by the large eddies from the mean flow and dissipated mostly at the smallest eddies through molecular viscous dissipation. Therefore, the turbulence kinetic energy dissipation rate is closely related to the molecular mixing. The turbulence kinetic energy divided by its dissipation rate, $k/e$, indicates a dissipation time scale. By dimensional argument we may estimate the dissipation rate of a general variable $\varphi$ as $c_{\varphi} \frac{\phi^{2}}{k}$ where $\varphi^{*} = \varphi^{2}$ and $c_{\varphi}$ is an empirical proportion coefficient.

Based on these arguments, the mean combustion rate can be estimated as $c_{\phi} \frac{\phi^{2}}{k}$, with $\phi$ representing the mass fraction.

For a general reaction represented by

$$aA + bB + cC + \cdots \rightarrow dD + eE + fF + \cdots$$  \hspace{1cm} (24)

where $a, b, c, d, e, f$ are the reaction coefficients, $A, B$ and $C$ represent the reactants (normally $A$ represents fuel), and $D, E$ and $F$ represent the products, assuming the fluctuation is simply related to the mean value, the mean reaction rate is modeled in EDC [9] by the turbulence dissipation rates of reactant and/or product eddies as

$$\bar{R}_A = -c_{\text{EDC}} \bar{\rho} \frac{c}{k} \min \left( \bar{Y}_A, \frac{a}{b} \bar{Y}_B, \frac{a}{c} \bar{Y}_C, \ldots \right)$$  \hspace{1cm} (25)
\( R_A = -c_{\text{EDC}} \frac{\varepsilon}{K} \min \left( \hat{Y}_A, \frac{a}{b} \hat{Y}_B, \frac{a}{c} \hat{Y}_C, \ldots, \frac{a}{d} \hat{Y}_D, \frac{a}{e} \hat{Y}_E, \frac{a}{f} \hat{Y}_F, \ldots \right) \) \hspace{1cm} (26)

where \( c_{\text{EDC}} \) is an empirical model constant. Usually, a value of about 4.0 can be used for \( c_{\text{EDC}} \) and in many cases the simulation is not very sensitive to the value used.

Obviously, the applicability of the above modeling procedure is limited by the introduced assumptions especially by the fast chemistry assumption. EDC was later extended [10] for possible inclusion of chemical kinetics, after introducing a series of assumptions.

2.1.3.2.2 Eddy dissipation concept in LES

The eddy dissipation concept was originally proposed for RANS. However, this concept can be easily extended for use in LES. In the modeled reaction rate formula shown in eqns (25) and (26), \( \frac{\varepsilon}{K} \) is the inverse of an estimated time scale. In LES, since neither \( k \) nor \( \varepsilon \) is computed, \( \frac{\varepsilon}{K} \) is not available. However, we can alternatively estimate the relevant time scale from the velocity field as \( 2/[((\partial \hat{u}/\partial x_i) + (\partial \hat{u}/\partial x_j))/((\partial \hat{u}/\partial x_i) + (\partial \hat{u}/\partial x_j))]^{0.5} \).

With the averaged variables replaced by corresponding filtered variables and the time scale replaced by the new estimation, eqns (25) and (26) can be used in a straight way to estimate the needed filtered reaction rates in LES.

2.1.3.2.3 Flamelet combustion model in RANS

Flamelet models provide another approach to deal with the closure problem created by pre-treating the non-linear reaction rates. In this section, flamelet combustion models will be presented for non-premixed combustion.

The structure of laminar diffusion flames has been found from measurements to be quite universal when it is plotted against the local equivalence ratio [35]. Assuming an infinitely fast chemistry, it can be shown that there exists a unique relation between mass fractions and mixture fraction for a two-stream system with equal mass diffusivities. When the chemistry is fast, but not infinitely fast, as it is in many practical considerations, to leading order the flame structure can still be regarded as well defined in a conserved scalar space, which is usually, but not necessarily, selected as the mixture fraction. Typically, the steady flamelet structure is given by \( Y_i = Y_i(f, \chi_{\text{st}}), T = T(f, \chi_{\text{st}}) \), where \( f \) is the mixture fraction, \( \chi \) is the scalar dissipation rate, and the subscript ‘st’ denotes stoichiometry. This flamelet structure can be obtained from detailed experimental measurements [35–37] or theoretical laminar flame calculations [38, 39].

The above discussion implies that in the modeling of turbulent non-premixed combustion, if we assume that the turbulent flame is an ensemble of laminar flamelets of well-defined structure, the detailed chemistry computation could be separated from the flow field calculation, and the modeling can proceed by finding out the flamelet statistics, which can be represented by a probability density function (PDF) \( \tilde{p}(f, \chi_{\text{st}}) \). The mean mass fraction in a turbulent flame is evaluated from the laminar flamelet structure and the statistics of the related conserved scalar and the scalar dissipation rate as

\[ \tilde{Y}_i = \int_0^\infty \int_0^\infty Y_i(f, \chi_{\text{st}}) \tilde{p}(f, \chi_{\text{st}}) \, df \, d\chi_{\text{st}} \] \hspace{1cm} (27)

If \( f \) and \( \chi_{\text{st}} \) are assumed statistically independent, then the above equation becomes

\[ \tilde{Y}_i = \int_0^\infty \int_0^\infty Y_i(f, \chi_{\text{st}}) \tilde{p}(f) \, df \frac{1}{\chi_{\text{st}}} \int_0^\infty \tilde{p}(\chi_{\text{st}}) \, d\chi_{\text{st}} \] \hspace{1cm} (28)
In a turbulent reacting flow the local PDF is very difficult to obtain but can be approximately prescribed or estimated from the solution of a carefully constructed PDF transport equation \([40-43]\). The prescribed PDF, \(\tilde{p}(f)\), can be constructed from the mean mixture fraction and its variance, for example, using the normalized beta \([12, 14, 17]\), clipped Gaussian function \([44]\) or top hat functions \([45]\). Very often, a prescribed normalized beta function PDF is used. The normalized beta function has only two parameters and can approximate reasonably well the usual PDF shape found in a jet when the parameters are properly given. In some situations, the simulation of a turbulent reacting flow may not be sensitive to the specific PDF shape \([45]\).

The PDF constructed using the normalized beta function can be written as

\[
p(f) = \frac{f_{\alpha-1}^{\alpha-1} (1-f)^{\beta-1}}{\int_0^1 f_{\alpha-1}^{\alpha-1} (1-f)^{\beta-1} df}
\]

where the function parameters \(\alpha\) and \(\beta\) can be related to the mean mixture fraction and its variance as \(\alpha = f_{\tilde{f}} (1-f_{\tilde{f}})/g_{\tilde{f}} - 1\), \(\beta = \alpha (1-f_{\tilde{f}})/f_{\tilde{f}}\), where \(g_{\tilde{f}}\) is the variance of the mixture fraction \(f_{\tilde{f}}^2\).

Both mean mixture fraction and its variance are given by the solution of their transport equations

\[
\frac{\partial(\tilde{f} \tilde{f})}{\partial t} + \frac{\partial(\tilde{f} \tilde{u}_j \tilde{f})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{f}}{\partial x_j} - \bar{p} u_{ij} \tilde{f} \right)
\]

\[
\frac{\partial(\tilde{g} \tilde{g})}{\partial t} + \frac{\partial(\tilde{g} \tilde{u}_j \tilde{g})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{g}}{\partial x_j} - \bar{p} u_{ij} \tilde{g} \right) - 2 \tilde{p} u_{ij} \tilde{f} \frac{\partial \tilde{f}}{\partial x_j} - c_e \tilde{g} \frac{\tilde{g}}{k}
\]

The third hypothesis of Kolmogorov states that the logarithm of the dissipation rate, averaged in a space much smaller than the integral scale, has a normal distribution \([2]\). Assuming a log-normal distribution of \(\chi\), the prescribed \(\tilde{p}(\chi)\) can be constructed as \([12, 14]\)

\[
\tilde{p}(\chi) = \frac{1}{\chi \sigma \sqrt{2\pi}} \exp \left\{ -\frac{1}{2\sigma^2} (\ln \chi - \mu)^2 \right\}
\]

where the parameters \(\mu\) and \(\sigma\) are related to \(\tilde{\chi}\) as

\[
\tilde{\chi} = \exp(\mu + 0.5\sigma^2)
\]

in which \(\sigma\) can be estimated from \(\sigma^2 = 0.5 \ln(0.1 Re^{0.5})\), and \(\tilde{\chi}\) can be modeled by

\[
\tilde{\chi} = c_e \frac{\tilde{g} \tilde{g}}{k}
\]

In this approach, the transport equation for the mean mass fraction is not solved and thus the mean reaction rate does not need to be directly modeled.

2.1.3.2.4 Flamelet combustion model in LES In LES, the flame is typically not spatially resolved and a SGS combustion model is needed to consider the interaction between turbulence and chemistry. The SGS models of non-premixed combustion based on the laminar flamelet concept are similar to the flamelet combustion models in RANS. At the SGS level, it is assumed that the turbulent flame is an ensemble of wrinkled laminar flamelets which have a well-defined structure. The interactions between turbulence and chemistry can be included...
by treating the turbulent reacting flow as a random process and introducing a SGS probability density function. Typically, as in RANS, a prescribed normalized beta PDF can be used. 

In order to parameterize the SGS normalized beta PDF, a modeled transport equation is solved to obtain the filtered mixture fraction $\tilde{f}$ and a scale-similarity model can be employed to determine the SGS mixture fraction variance $\tilde{g}$ [46].

The transport equation for the mixture fraction can be written as

$$\frac{\partial(\tilde{f})}{\partial t} + \frac{\partial(\tilde{u}_j \tilde{f})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc \tilde{f}} \frac{\partial \tilde{f}}{\partial x_j} + q_{j,f} \right)$$  \hspace{1cm} (35)

where $q_{j,f}$ is the SGS flux for mixture fraction which can be modeled as discussed in the LES turbulence modeling section.

The mixture fraction variance is given by

$$\tilde{g} = K (\tilde{f} - \bar{f})$$  \hspace{1cm} (36)

where $K$ is the model constant chosen as 3.0 [46].

In fires, the gas velocity is usually low (of the order of 1.0 m/s) and the local strain rate at the flame is low. If we assume that the effect of local extinction due to the flame stretch is of minor importance, the Favre spatially filtered mass fractions of the chemical species are then obtained from

$$\tilde{Y}_i = \int_0^1 Y_i(f) \tilde{f} \, df$$  \hspace{1cm} (37)

### 2.1.3.3 Soot modeling

Soot is of great interest for various reasons. The soot emitted from combustion poses a pollution threat to the environment and plays a role in smoke inhalation which is usually the main cause of death in fires. It can enhance the desired radiation heat transfer in industrial furnaces and the undesired radiation heat transfer in fires. Soot is also used as indication of fire in many fire detection systems.

Soot is a product of incomplete combustion of hydrocarbon fuels. In premixed flames, the hydrocarbon fuel will break into small hydrocarbon radicals when passing through the high temperature zone. From these radicals, small hydrocarbon molecules like acetylene can be formed. Under fuel rich conditions, the small molecules and radicals can react to form aromatic rings. Through ‘planar growth’ and coagulation, small soot particle nuclei can be formed from polycyclic aromatic hydrocarbons (PAHs). This process is the particle inception. The small particles that are formed will quickly coagulate and pick up gas phase component for surface growth. The coagulation determines the final soot particle size, while the surface growth is critical for the final soot volume fraction. The surface growth is mainly through the hydrogen abstraction carbon addition (HACA) mechanism and its rate is largely dependent on the number of active sites on the soot particle surface. The activity of soot particle surface can decrease quickly with residence time. The formed soot might be oxidized by O$_2$ and OH when transported to the lean region. The oxidation may be frozen when the temperature drops below about 1,300 K [47], and then the unoxidized soot will be emitted. In diffusion flames, the soot formation process is similar after the formation of the first ring. It is largely the initial stage that makes difference. In diffusion flames, since soot is formed in the fuel rich and relatively low temperature zone, the molecular structure of the parent fuel has more importance for soot tendency than in premixed flames [47, 48].
Detailed modeling of soot formation and oxidation is a prohibitive task. In general, despite significant progress in recent years [49], soot modeling is still in its infancy. For simple fuels, different flamelet-based soot models have been proposed. These models can work reasonably well when used with care within their limitations. In fires, normally involved is complex fuels such as woods and plastics. For these complicated fuels, one may still have to rely on empirical formulations to provide an approximate consideration of soot formation.

In the following sections, both the flamelet soot model and empirical soot model are presented. It should be noted that by taking the pre-treated variables respectively as averaged variables in RANS and filtered variables in LES, the presented soot models apply in the same form for both RANS and LES.

2.1.3.3.1 Flamelet-based soot model  Since surface growth and oxidation are heterogeneous slow processes, there is no strict state relation between the soot volume fraction and the mixture fraction and the classical flamelet concept is thus not applicable. However, it may be argued that the soot formation and oxidation rates can be approximated as a function of mixture fraction. Therefore, with the reaction source term provided, soot can be modeled within the framework of the flamelet concept by solving additional transport equations.

In recent years, a number of flamelet based soot models have been proposed. Moss has presented a two-variable soot model [50−53] which includes the essential physics. With the model parameters carefully adjusted through calibration, his model has been shown to be quite successful. A similar two-variable soot model was proposed by Lindstedt [54, 55] and was quite successfully applied to turbulent soot modeling [56, 57]. In this soot model, soot formation is related to the chemical intermediate acetylene rather than to the parent fuel which was used in the soot model suggested by Moss et al. [50−53]. Recently, Balthasar et al. [58] have presented a soot model in which the transport equation for soot volume fraction was solved with the source terms calculated in the mixture fraction/scalar dissipation rate space for laminar flamelets and tabulated in a library. In these models, based on the flamelet concept, the reaction rates of soot formation and oxidation are eventually considered as a function of mixture fraction alone. For brevity, the details of these models are not discussed here. Figure 6 shows preliminary result from a simulation of a C3H6 buoyant diffusion flame using Balthasar et al.’s soot model.

The application of the above-mentioned types of soot model is still limited to simple fuels. In [59], the flamelet soot model proposed by Lindstedt [54, 55] was employed for soot modeling in a CFD calculation of propane flame heat transfer. For complex fuels, as an estimation, simple empirical models based on measurements can be used [60, 61].

2.1.3.3.2 Empirical soot model  As stated before, for complicated fuels, one may still have to rely on empirical formulations to provide an approximate consideration of soot formation. This kind of empirical soot models can be constructed based on measurement data. For example, as an approximation, soot can be considered by assuming that a certain amount of fuel is simply converted to soot with an empirical soot conversion factor [60, 61] which can be chosen with reference to some experimental measurements. Different conversion factors should be used for different fuels. The soot conversion rate can be simply assumed to be locally proportional to either fuel supply rate or fuel combustion rate which can be modeled by the combustion model. The formed soot is subject to transport. A scalar transport equation is solved to calculate the soot mass concentration distribution. This transport equation can be written as

\[
\frac{\partial(\rho \hat{Y}_{\text{soot}})}{\partial t} + \frac{\partial(\rho \mathbf{u} \cdot \hat{Y}_{\text{soot}})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \hat{Y}_{\text{soot}}}{\partial x_j} - \frac{\rho \mathbf{u} \cdot \nabla \hat{Y}_{\text{soot}}}{Sc} \right) + \bar{R}_{\text{soot}} \quad \text{(for RANS)}
\]
In the above two equations, the conversion rate $R_{\text{soot}}$ can be modeled as $R_{\text{soot}} = c_{\text{conversion}} \times \text{(fuel supply rate)}$ or $R_{\text{soot}} = c_{\text{conversion}} \times R_{\text{fuel}}$ where $c_{\text{conversion}}$ is the empirical conversion factor and $R_{\text{fuel}}$ is the local fuel combustion rate which can be provided by the combustion model such as EDC.

2.1.3.4 Radiation modeling  Due to its strong dependence on temperature and the strong radiating behavior of combustion products, thermal radiation is an important heat transfer mechanism in many combustion systems, particularly in fires.

2.1.3.4.1 Radiation transfer equation (RTE) and its solution  Thermal radiation can be defined as electromagnetic waves emitted by a medium solely due to its temperature. The wavelength important to heat transfer is normally limited between 0.1 µm (ultraviolet) and 100 µm (mid-infrared). For a medium in local thermodynamic equilibrium, the differential equation of the spectral radiation can be written as [62, 63]

$$\frac{\partial I_{w,s}}{\partial s} = k_{w,s} I_{w,s}^0 - \beta_{w,s} I_{w,s} + \frac{\sigma_{w,s}}{4\pi} \int I_{w,s}(\vec{s},\vec{s}) \Phi(\vec{s},\vec{s^*}) d\Omega_i$$

where the superscript 0 stands for black body radiation, $k_{w,s}$ is the effective spectral absorption coefficient which represents induced transition including both induced absorption and induced emission, $\sigma_{w,s}$ is the spectral scattering coefficient, $\beta_{w,s}$ is the extinction coefficient $\beta_{w,s} = k_{w,s} + \sigma_{w,s}$, and $\vec{s}$ and $\vec{s^*}$ are the direction vectors, and $\Phi(\vec{s},\vec{s^*})$ is the phase function, which is equal to 1.0.
for isotropic scattering. The three terms on the right-hand side represent the augmentation due
to emission, the attenuation due to absorption and scattering, and the augmentation due to scat-
tering, respectively. Since the light speed in a medium is usually large, the radiation time scale is
much smaller than almost all the other practical time scales concerned in fires, the transient term
has been ignored in the above equation.

The spectral radiation transfer equation is usually rewritten using non-dimensional optical coor-
dinate as

$$\frac{\partial I_{w,i}}{\partial x_{w}} + I_{w,i} = (1 - \omega_{w})I_{w,i}^0 + \frac{\omega_{w}}{4\pi} \int I_{w,i}(\vec{s},\vec{s},) \Phi(\vec{s},\vec{s},) d\Omega = S_w(x_w,\vec{s})$$

(41)

where the single scattering albedo \(\omega_{w}\) is defined as \(\omega_{w} = \frac{\sigma_{s,i}}{\sigma_{w}}, x_w = I_0^1 \beta_{w,i} ds \) and the source func-
tion \(S_w(x_w,\vec{s}) = (1 - \omega_{w})I_{w,i}^0 + \frac{\omega_{w}}{4\pi} \int I_{w,i}(\vec{s},\vec{s},) \Phi(\vec{s},\vec{s},) d\Omega\).

The rewritten RTE is an integral–differential equation. Multiplying this RTE by \(e^{x_{w}}\) results in

$$\frac{\partial(I_{w,i}e^{x_{w}})}{\partial x_{w}} = S_w(x_w,\vec{s})e^{x_{w}}$$

(42)

which can be integrated along the radiation path from an arbitrary point \(s_1\) to another arbitrary
point \(s_2\) to give

$$I_{w,i}(x_{w},\vec{s})e^{x_{w}} = \int_{x_{w_1}}^{x_{w_2}} S_w(x_w,\vec{s})e^{x_{w}} dx_w + I_{w,i}(x_{w_1})e^{x_{w_1}}$$

(43)

This integration can be rewritten as

$$I_{w,i}(x_{w_2}) = \int_{x_{w_1}}^{x_{w_2}} S_w(x_w,\vec{s})e^{\left(x_{w_2} - x_{w_1}\right)} dx_w + I_{w,i}(x_{w_1})e^{\left(x_{w_2} - x_{w_1}\right)}$$

$$= \int_{x_{w_1}}^{x_{w_2}} S_w(x_w,\vec{s})e^{\left(x_{w_2} - x_{w_1}\right)} dx_w + I_{w,i}(x_{w_1})e^{\left(x_{w_2} - x_{w_1}\right)}$$

(44)

where \(e^{\left(x_{w_2} - x_{w_1}\right)}\) is the transmissivity from point \(s\) to point \(s_2\).

The above solution is a third order integral equation, where the source function itself is an
integration of unknown radiation intensity.

From the radiation intensity, the spectral heat flux vector and radiation energy source term
\((S_h\) in eqn (3)) can be readily calculated as

$$\vec{q}_w = \int \frac{I_w(\vec{s})}{4\pi} d\Omega$$

(45)

$$S_h = \nabla \cdot \vec{q}_w = \nabla \cdot \int \frac{I_w(\vec{s})}{4\pi} d\Omega = \int \frac{\partial I_w(\vec{s})}{\partial s} d\Omega = \int \frac{\partial I_w(\vec{s})}{\partial s} d\Omega$$

$$= \int \frac{r_{w,i}}{4\pi} I_w^0 - \beta_{w,i} I_{w,i} + \frac{\sigma_{w,i}}{4\pi} \int I_w(\vec{s},\vec{s},) \Phi(\vec{s},\vec{s},) d\Omega$$

$$= k_{w,i} \left(4\pi I_w^0 - \int I_w(\vec{s}) d\Omega\right)$$

(46)
Due to its complexity, an exact solution for radiation can only be obtained for a few simple cases. For most practical applications where the radiation path is usually non-gray and non-homogeneous, solutions are obtained using engineering approximation methods.

There are a number of approximate methods to solve the RTE and obtain $S_R$ and the radiation heat flux to surfaces, including the spherical harmonics method ($P_N$ approximation), the discrete ordinates method, the discrete transfer method, the finite volume method, the zonal method and the Monte Carlo method. The discussion of these methods can be found in [63, 64].

Since radiation has a highly non-linear dependence on the radiating medium’s thermal properties including temperature and mass compositions, the pre-treatment of the radiation within the RANS and LES concepts is extremely complicated. As an approximation, in normal practice, the mean/filtered radiation flux and radiation energy source term are modeled simply based on radiating medium’s mean/filtered thermal properties.

2.1.3.4.2 Radiation property evaluation

The radiation properties of the radiating medium must be evaluated when solving the radiation equation. Commonly adopted radiation property evaluation methods are the total absorptivity method [65], the weighted sum of gray gas (WSGG) method [65], the spectral line weighted sum of gray gas (SLWSGG) [66] method, the wide band model [67], and the narrow band model [68].

In fires, radiation comes from both gases and particles. The radiating gases normally include water vapor, carbon dioxide, hydrocarbon fuels, and carbon monoxide, etc. The particles mainly include soot.

Radiating gas and soot have quite different radiation behavior. At the moderate temperature, in the gas, bound-free and free–free transitions are rare and the energy level transitions mainly happen as bound–bound transition. According to quantum theory, the molecular energy levels are quantitized. As a result, the radiating gases are highly non-gray showing strong band radiation. Water vapor and carbon dioxide are usually the main radiating gases in a combustion system, having their most important infrared radiation bands centered at 1.38, 1.87, 2.7, and 6.3 microns for water vapor, 2.7 and 4.3 microns for carbon dioxide. The diatomic molecules including oxygen and nitrogen do not radiate at normal combustion temperature. In some situations, the gas fuels and their intermediates may play an important role in radiation. According to Mie’s scattering theory, the scattering efficiency factor is proportional to the fourth power of the particle’s size parameter. Since the gas molecules are much smaller than the thermal radiation wavelength, their contribution to the scattering is negligible.

Soot particle radiation includes both scattering and absorption/emission, but the scattering can also be ignored when the particle is sufficiently small. Soot shows a spectrally continuous radiation and is quite gray since its spectral absorption coefficient is a weak function of the wavelength (approximately proportional to the inverse of wavelength when the particles are small).

Spectral radiation of gases: The spectrum of a radiating gas consists of a large number of individual radiation lines. Each individual line corresponds to a transition between two molecular quantitized energy levels. However, the individual line is not exactly monochromatic. It is broadened by nature broadening, collision broadening, and Doppler broadening. Thus, each individual line has some finite width. The shape of collision broadened line is the same as that of nature broadened line, but differs from that of Doppler broadened line. The width of the broadened line is dependent on the broadening mechanism and the mixture’s thermal state. Since collision broadening results from molecule’s collisions which are proportional to molecule’s number density (proportional to $n$) and average speed (proportional to $\sqrt{T}$), it is not surprising that the half-width of the collision line is proportional to $n \sqrt{T}$. The Doppler line’s half-width is, on the contrary, proportional to $\sqrt{T}$ and the wave number. When calculating radiation, all the broadening
mechanisms should be considered in principle. But in many cases the collision broadening is much more important and the problem can be simplified. When the collision line’s half-width is 2 or 3 times more than that of the Doppler line, the Doppler broadening can be ignored. At high temperature and/or low pressure, due to the different variation behaviors of the half-widths of collision and Doppler lines, and that the shift of the important part of Planck function to large wavenumber spectrum, the Doppler line can become important.

**Spectral radiation of soot particle:** The radiation behavior of soot particles varies with the chemical composition of the particle. This variation can be very complex, and is thus often ignored. Assuming the soot particles are sufficiently small so that the scattering can be ignored, we have [63]

$$Q_{\text{abs}} = -4\pi r^2 \left( \frac{m^2 - 1}{m^2 + 2} \right) \cdot \frac{2\pi r}{\lambda}$$

(47)

$$k_\lambda = \int_0^\infty \pi r^2 n_p(r) Q_{\text{abs}} dr = -63 \left( \frac{m^2 - 1}{m^2 + 2} \right) \int_0^\infty \frac{4}{3} \pi r^3 n_p(r) dr$$

(48)

where $Q_{\text{abs}}$ is the absorption efficiency factor, $r$ is the radius of the idealized spherical particle, $n_p(r)$ is the particle number density, $\Im$ denotes the imaginary part, and $\int_0^\infty \frac{4}{3} \pi r^3 n_p(r) dr$ gives the soot volume fraction $f_v$.

The above equation can further be written as

$$k_\lambda = -3 \left( \frac{m^2 - 1}{m^2 + 2} \right) \frac{6\pi f_v}{\lambda} \approx \frac{36\pi nk}{(n^2 - k^2 + 2)^2 + 4n^2 k^2}$$

(49)

which indicates that the spectral radiation absorption coefficient of a soot cloud of small particles is proportional to the soot volume fraction and inversely proportional to the wave length.

The complex refractive index is dependent on the particle’s chemical composition, which is expected to vary with fuel type. Hottel and Sarofim [65] suggested a value of about 7.0 for $\frac{36\pi nk}{(n^2 - k^2 + 2)^2 + 4n^2 k^2}$. Therefore, we approximately have $k_\lambda = 7.0 \frac{f_v}{\lambda}$.

**Narrow band model for a constant parameter path:** The spectrum of a radiating gas is usually highly complex. Although the exact solution of gas radiation can be obtained in principle by line-by-line calculations, it requires a huge computation effort and all the detailed information of the individual lines, and is thus prohibitive. This problem necessitates model approximations. The narrow band model is the most accurate engineering method for the evaluation of radiation properties. In the narrow band model, the evaluation is carried out not on every individual line but on small spectrum intervals which are normally at 5−50 cm$^{-1}$. Within each narrow band, there are many individual lines. Therefore, the purpose of narrow band models is to approximate the mean radiation properties within the small spectrum intervals. In order to extract their mean radiation properties, the information about the strength distribution, spacing, width, and shape of the individual lines are needed. This information usually turns out to be very complicated. As a result, approximations are introduced when constructing the narrow band models. The line broadening mechanism describes the line shape and its width. Most important assumptions are related to line strength distribution and line spacing. Different approximations on line distribution and line spacing result in different narrow band models. The choice of a specific narrow band model can be based on accuracy and mathematical simplicity. The accuracy of a particular narrow band model relies on how well its assumptions comply with the spectrum structure of the radiating.
molecule being considered. The regular model (Elasser model) is more appropriate for simple molecules which have approximately equal line spacing and line strength, particularly when the Q branch is not important or even presented. For complex molecules which have irregular line strength distribution and line spacing, the random (statistical) model can be more applicable.

The spectral absorption coefficient at any wavenumber can be calculated as a sum of the contributions from all the individual lines

$$k_w = \sum_n k_{wn}.$$  \hspace{1cm} (50)

The mean spectral (narrow band) absorption coefficient and emissivity can be calculated from

$$\bar{k}_w = \frac{1}{\Delta w} \int_{w-\frac{\Delta w}{2}}^{w+\frac{\Delta w}{2}} k_w \, dw'. \hspace{1cm} (51)$$

$$\bar{\varepsilon}_w = \frac{1}{\Delta w} \int_{w-\frac{\Delta w}{2}}^{w+\frac{\Delta w}{2}} \left[ 1 - \exp \left( -\frac{1}{0} \int_{0}^{s} \bar{k}_w \, ds \right) \right] \, dw'. \hspace{1cm} (52)$$

Since \(\varepsilon\) is a non-linear function of \(\bar{k}\), \(\bar{\varepsilon}_w\) cannot be simply written as \(\varepsilon_w(\bar{k}_w)\), even for a homogeneous and isothermal path. This is similar to the problem found in turbulent combustion modeling where the mean reaction rates cannot be given solely by the mean temperature and mean concentrations.

Narrow band models give approximations for \(\bar{k}_w\) and \(\bar{\varepsilon}_w\). Depending on the approximation of line distribution, different narrow band models can be proposed. In particular, the following discussion of FASTNB and approximate FASTNB is based on a narrow band model where the so-called Goody model is adopted for the collision line and a random model of equal line strength is adopted for Doppler line [68].

**Fast narrow band (FASTNB) model:** The narrow band model is the most accurate engineering approximation method, but it is usually expensive to implement. The computation speed of narrow band computations is of critical importance. In [69], a FASTNB computer model which predicts the radiation intensity in a generally non-isothermal and non-homogeneous combustion environment was developed.

Due to the complexity of the radiation, there is no analytical expression for the narrow band calculation of the radiation intensity. Therefore, the calculation must rely on a numerical solution. The line path is broken into a number of elements and the thermal radiation spectrum is divided into many (several hundred) small intervals. The spectral and spatial integrations are thus replaced by summations over all the spectrum intervals and elements, respectively. The radiation transfer equation then becomes

$$I = \sum_{m=1}^{M} I_{w_m} \Delta w_m = \sum_{m=1}^{M} \sum_{j=1}^{N} I_{w_m,j}^{0} \left( \tau_{w_m,j \rightarrow N} - \tau_{w_m,j \rightarrow 1} \right) \Delta w_m. \hspace{1cm} (53)$$

The main task is to calculate the transmissivity \(\tau_{w_m,j \rightarrow N}\). In the narrow band equations, in the evaluation of transmissivity, there are two important band parameters, \(\bar{S}/d\) and \(1/d\). These two parameters are functions of both temperature and wavenumber, and can be evaluated by molecular models or by interpolation from tabulated data. This evaluation consumes a large amount
of CPU time and it is repeated in the case of non-homogeneous paths with multiple elements. The CPU time would significantly be reduced if this evaluation could be avoided. One possible method of doing this is to pre-evaluate these two parameters and create a once-and-for-all database for them [69].

As mentioned above, the thermal radiation spectrum is divided into many intervals. We can now compute the band parameters \( S/d \) and \( 1/d \) in advance at all these corresponding discrete wavenumbers and temperatures, by the molecular model or the interpolation of tabulated data. Therefore, a once-and-for-all database can be created for both \( S/d \) and \( 1/d \). In the computer program, the data for each parameter can be stored in a two-dimensional array and can be used directly.

By pre-creating a database, the evaluation of band parameters can be avoided during narrow band calculations and the computation speed can be significantly improved.

FASTNB provides an accurate calculation at reasonably fast speed. When compared with Grosshandler’s narrow band model RADCAL [70], which has been verified quite extensively against experimental measurements, FASTNB is substantially faster and gives almost exactly the same result as RADCAL, as shown in Fig. 7.

The details of FASTNB can be found in [69].

*Approximated fast narrow band (approximated FASTNB) model:* The approximated FASTNB was developed in [71] to further speedup the narrow band model computations at a price of small loss in accuracy. Considering a calculation of spectral radiation intensity along a single radiating path which is spatially discretized into \( N \) elements in a narrow band model including FASTNB since the non-gray effects in a narrow spectral interval are modeled, in order to calculate the spectral radiation intensity \( I_{w,n} \) for the \( n \)th element of the path according to eqn (53), there will be \( n \) evaluations of spectral transmissivity. Therefore, to compute a complete radiation intensity distribution along the whole path, the total number of the spectral transmissivity evaluation along this radiating path will be

\[
1 + 2 + 3 + \cdots + N = (1 + N) \times N / 2
\]

which is proportional to \( N^2 \).

![Figure 7: Comparison of total intensities, for a path of parabolic minimum temperature and concentrations, with a uniform soot volume fraction of \( 2.0 \times 10^{-6} \) [69] (©Taylor & Francis).](image-url)
Assuming locally gray behavior in a small spectral interval in each spatial element which has a local mean spectral absorption coefficient $\bar{k}_{m,n}$, the computational effort can significantly be reduced to be proportional to $N$. In this case, the spectral transmissivity $\tau_{w_{n-1} \rightarrow n}$ can be approximated as follows

$$
\tau_{w_{n-1} \rightarrow n} = \exp\left(-\sum_{i=j}^{n} \bar{k}_{w_{n-1}u_i}\right) = \exp\left(-\sum_{i=j}^{n-1} \bar{k}_{w_{n-1}u_i}\right) \times \exp(-\bar{k}_{w_{n}u_n}) \\
= \tau_{w_{n-1} \rightarrow n-1} \exp(-\bar{k}_{w_{n}u_n}) = \tau_{w_{n-1} \rightarrow n-1}\tau_{w_{n-1} \rightarrow n-2}
$$

(55)

Therefore, we have

$$
I_{w_{n}} = \sum_{j=1}^{n} I_{w_{n-1}}^{0} (\tau_{w_{n-1} \rightarrow n} - \tau_{w_{n-1} \rightarrow n-1}) \\
= \sum_{j=1}^{n-1} I_{w_{n-1}}^{0} (\tau_{w_{n-1} \rightarrow n} - \tau_{w_{n-1} \rightarrow n-1}) + \sum_{j=n}^{n} I_{w_{n-1}}^{0} (\tau_{w_{n-1} \rightarrow n} - \tau_{w_{n-1} \rightarrow n-1}) \\
= \sum_{j=1}^{n-1} I_{w_{n-1}}^{0} (\tau_{w_{n-1} \rightarrow n-1} - \tau_{w_{n-1} \rightarrow n-1}) \times \exp(-\bar{k}_{w_{n}u_n}) + I_{w_{n-1}}^{0} (1.0 - \tau_{w_{n-1} \rightarrow n-1}) \\
= I_{w_{n-1}}^{0} \tau_{w_{n-1} \rightarrow n} + I_{w_{n-1}}^{0} (1.0 - \tau_{w_{n-1} \rightarrow n})
$$

(56)

which shows that the spectral intensity for a spatial element $n$ is directly related to the spectral intensity for the spatial element $n-1$. If we march the computation along the radiating path from spatial element 1 to element $N$, for each element, we will only need to evaluate one new local spectral transmissivity. As a result, the total computational effort on spectral transmissivity evaluation is linearly proportional to $N$.

The local spectral transmissivity can still be evaluated using the same formulas as those in the original narrow band model [71].

The deviation caused by the approximation is analyzed in [71]. In general, we can expect the loss in accuracy in the calculated radiation intensity to be small, particularly when a radiating path is contaminated by soot. Figures 8 and 9 show comparisons between the approximate FASTNB and FASTNB models for typical paths.

As analyzed before, the computational effort is proportional to $N^2$ in the original FASTNB and to $N$ in the FASTNB approximation. This implies that the speedup will approximately increase linearly with $N$. This can clearly be seen in Fig. 10. Therefore, a high speedup ratio can be expected in a heavy computation where $N$ is large.

More details about the FASTNB approximation can be found in [71].

2.2 Modeling of the response of solid materials

In conventional fires, the bulk solid material responds and feeds back to the state variation of its surrounding gases. For a combustible solid material, the most important processes inside the solid include both heat conduction and pyrolysis, which will be discussed in the following sections. In most cases, simulation of a conventional fire is of interest only during the fire period before flashover. During this short period, for each surface of a solid exposed to fire, the heat
wave penetration is limited to a thin layer (usually less than a few centimeters). In the following sections, for convenience of discussion, we generally denote such a surface layer as a wall. Please note that such a general wall can but does not have to be a real building wall. It can represent for example the surface layer of a wood table.

Figure 8: Comparison of total intensities, 50 spatial cells along the path, without soot [71] (©Taylor & Francis).

Figure 9: Comparison of total intensities, 50 spatial cells along the path, with uniform soot volume fraction of $20 \times 10^{-6}$ [71] (©Taylor & Francis).
2.2.1 Heat conduction inside a solid wall

Heat conduction inside a wall determines the internal temperature distribution and provides the necessary boundary condition for the gas phase calculation. For an inert wall, the heat balance is described by the following transient heat conduction equation

\[
\frac{\partial (\rho H)}{\partial t} = \nabla \cdot (k \nabla T) \tag{57}
\]

where \( H \) is the enthalpy given by \( H = H_0 + \int_{T_0}^{T} c_p dT \). The specific heat \( c_p \) and conductivity \( k \) are usually temperature dependent and can be represented by polynomial functions.

In a typical conventional fire such as a building fire, the walls of interest are usually connected and each wall is exposed to gas on two surface sides. In principle, the heat conduction should be considered in three-dimensional space with coupling between walls included. However, simplifications can usually be made. In many cases, the heat conduction from one wall to another through their inter-connection is of minor importance in comparison with the heat transfer between the wall and its surrounding gas. Furthermore, if the heat conduction along the direction perpendicular to wall surface dominates the problem can further be simplified to be one-dimensional. Consequently, the multidimensional heat conduction equation reduces to its one-dimensional form, which is

\[
\frac{\partial (\rho H)}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \tag{58}
\]

The initial and boundary conditions can be given by

\[
T(t = 0, x) = T_0(x) \tag{59}
\]

\[
k \frac{\partial T}{\partial x} \bigg|_{\text{surface}} = h_c (T_{\text{gas}} - T_{\text{surface}}) + R_{\text{flux}} \tag{60}
\]
where $R_{\text{flux}}$ represents the net radiation flux, $T_{\text{gas}}$ is the temperature of the gas close to the wall surface, and $h_c$ is the convection heat transfer coefficient. These parameters are provided by the gas phase modeling of turbulent combustion. Due to space limitations, the important convective heat transfer is not included in the above discussion of turbulent combustion modeling. Normally because the boundary layer is very thin and it is very expensive to resolve the boundary layer in simulations, the convective heat transfer is calculated using wall functions. Information on wall functions and their application in calculating convective heat transfer in fire simulation can be found in [61, 72, 73] and the references cited therein.

When a solid wall is exposed to fire, it may be subjected to intensive heating. Meanwhile, most practical solid wall materials are not good heat conductors. Along the direction perpendicular to the wall surface, the temperature gradient in a solid can be very high particularly near the wall surface. The accuracy requirement of the numerical solution of this heat conduction equation necessitates adoption of a grid which can be much finer (typically around 1.0 mm) than that used in the gas phase computation. Therefore, the presently affordable gas phase numerical grid cannot be directly adopted for solid phase computations and a separate grid system is needed for the solid phase calculation. In the simplified one-dimensional case, the surface of a wall is subdivided into many small elements according to the gas phase grid and along the direction which is perpendicular to the surface each element is represented by a number of thin slices which can be less than 1 mm thick. Therefore, a special grid arrangement needs to be made where separate grids are used for the gas phase computation and the solid phase temperature calculation. Figure 11 illustrates a grid system which can be adopted. In this grid system, the surface of a solid boundary is subdivided into many small elements according to the gas phase grid, and along the direction perpendicular to the surface, each element is represented by a number of very fine slices used for solid calculation.

2.2.2 Pyrolysis modeling
In conventional fires, many involved solid walls are combustible. When sufficiently heated, these combustible walls start to degrade and pyrolyze. Since the pyrolysis is usually highly complex, the detailed pyrolysis modeling of solid fuels is a very difficult task. Fortunately, in fire simulations 

![Figure 11: Illustration of a separate grid system [74] (©Taylor & Francis).](image-url)
particularly when the energy output is of major concern the pyrolysis modeling can be simplified without losing the main physics.

The pyrolysis reaction can be described in a simplified form as:

Virgin material → Volatile products + Char

For a non-charring material, char will not be produced during the pyrolysis.

For a pyrolyzing material, in a local very small finite volume represented by a control volume used in numerical computation, virgin material, char, and volatile products may coexist. If we denote their volume fractions by $\gamma_{\text{vir}}$, $\gamma_{\text{char}}$, and $\gamma_{\text{vol}}$, respectively and assume one-dimensional mass flow along the direction perpendicular to the wall surface, considering that chemical reactions do not affect the total enthalpy in a reacting system, the energy balance equation in a pyrolyzing material can be written as:

$$\frac{\partial (\rho_{\text{vir}} \gamma_{\text{vir}} h_{\text{vir}} + \rho_{\text{char}} \gamma_{\text{char}} h_{\text{char}} + \rho_{\text{vol}} \gamma_{\text{vol}} h_{\text{vol}})}{\partial t} + \frac{\partial (m'' h_{\text{vol}})}{\partial x} = \nabla \cdot (k \nabla T) \quad (61)$$

where the subscripts vir, char, and vol denote the virgin material, char, and volatile products, respectively, $x$ is the coordinate along the direction perpendicular to the wall surface, $h$ is the total enthalpy, and $m''$ is the mass flux of the volatile products. The three terms in the above equation represent the energy storage, energy convection due to the flow of the volatile products, and heat conduction, respectively. The effects of pressure variation and flow kinetic energy are ignored.

The above equation can be reorganized as:

$$\frac{\partial (\rho_{\text{vir, bulk}} h_{\text{vir}} + \rho_{\text{char, bulk}} h_{\text{char}} + \rho_{\text{vol, bulk}} h_{\text{vol}})}{\partial t} + \frac{\partial (m'' h_{\text{vol}})}{\partial x} = \nabla \cdot (k \nabla T) \quad (62)$$

where $\rho_{\text{vir, bulk}} = \rho_{\text{vir}} \gamma_{\text{vir}}$ is the local bulk density of virgin material, $\rho_{\text{char, bulk}} = \rho_{\text{char}} \gamma_{\text{char}}$ is the local bulk density of char, and $\rho_{\text{vol, bulk}} = \rho_{\text{vol}} \gamma_{\text{vol}}$ is the local bulk density of volatile products.

As already mentioned, in many cases, the heat conduction along the direction perpendicular to the wall surface dominates and can thus be simplified to one-dimensional as well. The above energy balance equation then becomes:

$$\frac{\partial (\rho_{\text{vir, bulk}} h_{\text{vir}} + \rho_{\text{char, bulk}} h_{\text{char}} + \rho_{\text{vol, bulk}} h_{\text{vol}})}{\partial t} + \frac{\partial (m'' h_{\text{vol}})}{\partial x} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right). \quad (63)$$

For convenience, the discussion that follows will be based on the above equation with one-dimensional heat conduction. However, it is straightforward to extend the discussion to a case with three-dimensional heat conduction.

The mass conservation gives:

$$\frac{\partial (\rho_{\text{vir, bulk}} + \rho_{\text{char, bulk}} + \rho_{\text{vol, bulk}})}{\partial t} + \frac{\partial m''}{\partial x} = 0 \quad (64)$$

For simplicity, we assume an instant escape of the volatile products from the solid. Thus, we have $\frac{\partial \rho_{\text{vol, bulk}}}{\partial t} = 0$ and $\rho_{\text{vol, bulk}} = 0$. If we further write $\rho_{\text{vir, bulk}} + \rho_{\text{char, bulk}}$ as $\rho$, and assume $h_{\text{vir}} = h_{\text{char}} = h_s$, where the subscript $s$ denotes the solid, the above two equations can be rewritten as:

$$\frac{\partial (\rho h_s)}{\partial t} + \frac{\partial (m'' h_{\text{vol}})}{\partial x} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \quad (65)$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial m''}{\partial x} = 0 \quad (66)$$
Combining eqns (65) and (66) gives
\[
\frac{\partial}{\partial t} \left[ \rho_s (h_s - h_{s,0}) \right] + \frac{\partial}{\partial x} \left[ \dot{m}''(h_{\text{vol}} - h_{s,0}) \right] = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \tag{67}
\]
where \( h_{s,0} \) is the total enthalpy of the solid at a reference temperature \( T_0 \) and \( h_s - h_{s,0} \) is the sensible enthalpy given by \( h_s - h_{s,0} = \int_{T_s}^{T_0} c_p \, dT \). For convenience, we define \( H_s = h_s - h_{s,0} = \int_{T_s}^{T_0} c_p \, dT \) and similarly \( H_{\text{vol}} = h_{\text{vol}} - h_{\text{vol},0} = \int_{T_s}^{T_0} c_{p,\text{vol}} \, dT \).

The total enthalpy of volatile products can be written as
\[
h_{\text{vol}} = h_{s,T_s} + H_{py} + \int_{T_s}^{T_p} c_{p,\text{vol}} \, dT = h_{s,T_s} + H_{py} + H_{\text{vol},T_s} - H_{\text{vol},T_p} \tag{68}
\]
where \( H_{py} \) is the chemical conversion heat associated with a unit mass of volatile products, and can be calculated by the difference in total enthalpy of the virgin material and the volatile products at temperature \( T_p \), i.e.
\[
H_{py} = h_{\text{vol},T_p} - h_{s,T_s} = h_{\text{vol},T_p} - h_{\text{vir},T_s} = h_{\text{vol},T_p} - \left( h_{s,T_s} + \int_{T_s}^{T_p} c_{p,\text{vir}} \, dT \right) \tag{69}
\]
It is worth pointing out that \( H_{py} \) is approximately constant for a specific material and is different from the heat of gasification, \( H_g \), where
\[
H_g = \frac{\dot{q}_{\text{net}}}{\dot{m}_{\text{total}}} = \frac{h_t (T_s - T_{x=0}) + R_{\text{flux}}}{\dot{m}_{\text{total}}} \tag{70}
\]
which is a local and transient value and changes considerably during the pyrolysis process [75]. For the thermally thick vaporizing material, at steady state
\[
H_g = h_{\text{vol},T_p} - h_{\text{vir},T_s} = H_{py} + \int_{T_s}^{T_p} c_{p,\text{vir}} \, dT. \tag{71}
\]
Using eqn (68) and \( h_{s,T_s} = h_{s,0} + H_{s,T_s} \), the left-hand side of eqn (67) can be reorganized as
\[
\frac{\partial}{\partial t} \left[ \rho_s (h_s - h_{s,0}) \right] + \frac{\partial}{\partial x} \left[ \dot{m}''(h_{\text{vol}} - h_{s,0}) \right] = \frac{\partial}{\partial x} \left[ \dot{m}''(H_{s,T_s} + H_{py} + H_{\text{vol},T_s} - H_{\text{vol},T_p}) \right] \tag{72}
\]
where \( \dot{m}'' = \frac{\partial m''}{\partial x} \), representing the mass loss rate of the pyrolyzing material per unit volume.
Since the pyrolysis happens in a narrow temperature range around $T_p$, $H_s$, $T_p$ can be approximated by $H_s$ when $\dot{m}^{mm}$ is of importance, we can therefore rewrite the above equation approximately as

$$\frac{\partial (\rho H)}{\partial t} + \dot{m}^{mm}(H_{py} + H) + \frac{\partial}{\partial x}\left[\dot{m}^{mm}(H_{vol} - H_{vol,T_p})\right] = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$$

(73)

where the third term is the energy required to heat the vaporized gas as it flows to the solid surface. This term has no important effect here, thus it will be ignored. But it can be very easily included.

From the mass conservation equation and the definition $\dot{m}^{mm} = \frac{\partial m^{\infty}}{\partial x}$, one can have

$$\dot{m}^{mm} = -\frac{\partial \rho}{\partial t}$$

(74)

Noting that $\frac{\partial (\rho H)}{\partial t} = H \frac{\partial \rho}{\partial t} + \rho \frac{\partial H}{\partial t} = H \frac{\partial \rho}{\partial t} + \rho c_p \frac{\partial T}{\partial t}$ and $\dot{m}^{mm} = \frac{\partial m^{\infty}}{\partial x}$, the energy equation can be rewritten as

$$\rho c_p \frac{\partial T}{\partial t} + \dot{m}^{mm} H_{py} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$$

(75)

Assumptions have been introduced during the derivation of the simplified energy conservation equation. These assumptions can be better justified for non-charring materials. To be more general, assumptions can be lifted at the expense of increasing the complexity.

The eqns (74) and (75) are the final mass conservation and energy conservation equations to be solved for modeling of pyrolysis.

To implement the numerical solution, eqn (75) needs to be discretized first. The discretization can be based on either an implicit or explicit scheme. When the pyrolysis model is coupled with CFD for flame spread simulations, the time marching scheme in the pyrolysis model should fit with the time marching scheme in CFD. Typically, for the pyrolysis model, an implicit scheme is used when the RANS CFD concept is employed and an explicit scheme is adopted when the LES CFD concept is used.

For convenience, we will present the discussion with one typical discretization which is based on the fully implicit backward time stepping and the central space difference scheme. With this typical discretization, the discretized energy equation can be written as

$$\rho c_p \frac{T_n - T_n'}{\Delta t} \delta x + m_{\delta x}^{\infty} H_{py} = k_{(n+1)(n)} \frac{T_{n+1} - T_{n}}{\delta x} - k_{(n)(n-1)} \frac{T_n - T_{n-1}}{\delta x}$$

(76)

where the prime indicates the previous time step, $m_{\delta x}^{\infty}$ is the mass loss rate per unit area of the $\delta x$ thick strip, and the subscript of the conductivity $k$ denotes the two temperature nodes between which the surface of the control volume is located.

For convenience, we reorganize the above discrete equation as

$$A_e T_n = A_w T_{n+1} + A_w T_{n-1} + S_u$$

(77)

where

$$A_e = \frac{k_{(n+1)(n)}}{\delta x}, \quad A_w = \frac{k_{(n)(n-1)}}{\delta x}$$

(78)

$$A_p = A_e + A_w + \rho c_p \delta x / \Delta t$$

(79)
Since the conductivity, $k$, is generally a function of temperature, it may vary with $x$ and it is not necessary for $A_e$ to be equal to $A_w$.

In order to get a reasonable result for the mass loss rate, a very fine grid was required to resolve the density profile in the pyrolyzing layer and locate the pyrolysis front. However, this very fine grid is unnecessary and very expensive for the temperature solution. This inconsistency is overcome by introducing a dual mesh concept where a relatively coarser grid is defined for the temperature solution and then refined into a second grid for the mass loss rate calculation, as shown in Fig. 12.

The temperature of the refined grid $m$ of the coarser grid $n$ (we will denote this grid as grid $(n,m)$ later), $T_{n,m}$, is obtained by interpolation, as shown in Fig. 12, assuming a linear distribution between $T_n$ and $T_{n+1}$.

In the above discussion, the mass and energy balance equations and their discretizations are presented. However, from the mass and energy balance equations, one can easily find out that in these two equations, there are three dependent variables, namely $r$, $\dot{m}^m$, and $T$. The equation system is not closed. This is because the pyrolysis chemistry is not yet considered to relate the mass loss rate $\dot{m}^m$ with the other two dependent variables. As presented below, depending on how the mass loss rate $\dot{m}^m$ is evaluated with $r$ and $T$, one can basically have two different pyrolysis modeling procedures within the above overall framework.

**2.2.2.1 Thermo-pyrolysis modeling** For most combustible solid materials, the activation energy of the pyrolysis is large [76]. Due to the large activation energy and the endothermic feature of the pyrolysis process, the pyrolysis mainly happens in a narrow temperature range. The approximate constancy of the pyrolysis temperature suggests that below the pyrolysis temperature $T_p$, the pyrolysis reaction proceeds at a negligible rate, but above the pyrolysis temperature, the chemistry becomes so fast that the pyrolysis rate is then essentially determined by the physical heat transfer. Therefore, as far as the mass release rate is concerned, the pyrolysis can well be described by the heat balance without the need of going to the details of the chemical reaction rates which may involve many unknown chemical mechanism parameters.

![Figure 12: Temperature solution grid and its refinement (e.g. with $N = 5, M = 10$, where $N$ is the coarser grid number and $M$ is the refined grid number in a coarser grid) [60] (©Elsevier Science Ltd., with permission).](image-url)
As mentioned before, the pyrolysis rate is slow when the material temperature is below its pyrolysis temperature, $T_p$, and becomes fast when the temperature is above $T_p$. As an approximation, we can reasonably assume that the material will start to pyrolyze only when its temperature reaches the pyrolysis temperature.

Once started, the endothermic pyrolysis process will adjust its rate to keep the material temperature at the pyrolysis temperature until the material is completely pyrolyzed.

Thus we have

$$\rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \quad \text{when} \quad T \leq T_p \quad \text{or} \quad \rho = \rho_{\text{char}}$$

$$m'' H_{\text{py}} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \quad \text{when} \quad T \geq T_p \quad \text{and} \quad \rho > \rho_{\text{char}}$$

During the iteration, $T_{n,m}$ may exceed the pyrolysis temperature. In and only in this case, the endothermic pyrolysis will be induced and then it will adjust itself to limit the local temperature to the pyrolysis temperature. Thus, from eqn (77), for an arbitrary refined grid $(n,m)$, the energy available for pyrolysis can be approximated as

$$H_{n,m} = \max \left\{ 0,0, A_p (T_{n,m} - T_p) / M \right\}$$

where $M$ has been defined in Fig. 12.

The above energy excess allows the pyrolyzing layer to spread over a number of refined grids and provides one necessary, but not sufficient, factor to determine the pyrolysis rate.

In order to finally calculate the pyrolysis rate, one also needs to know the mass of the volatile material remaining in the refined grid $(n,m)$. The volatile mass remaining in a refined grid can be easily calculated by monitoring its density history. However, this would require much memory storage, particularly when dealing with a large number of pyrolyzing solid elements in flame spread simulations. In order to minimize the memory usage and make the data structure of the computer program more tidy, only the variation of the average density of the coarser grids is followed. The density of a refined grid is calculated by assuming a specific density distribution in the coarser grid. For a coarse temperature grid of an average density which is equal to $\rho_{\text{char}}$ or $\rho_{\text{vir}}$, the density of its refined grid will simply be the same as the average density. For a partly pyrolyzed coarser grid, if we assume that the char layer and the virgin material is separated by a single partly pyrolyzed refined grid, the density of a refined grid will be either $\rho_{\text{char}}$, $\rho_{\text{vir}}$ or $\rho_{\text{mix}} = M \rho - (m_0 - 1) \rho_{\text{char}} - (M - m_0) \rho_{\text{vir}}$ in the $\rho_{\text{mix}}$ formula, $\rho$ is the average density of the coarse temperature grid, the integer $m_0$ locates the assumed partly pyrolyzed refined grid and can be determined by requiring $\rho_{\text{mix}} < \rho_{\text{mix}} < \rho_{\text{vir}}$.

For an arbitrary refined grid $(n,m)$, the density can be generalized by a single formula

$$\rho_{n,m} = \min \{ \rho_{\text{vir}}, \max (\rho_{\text{char}}, \rho_{\text{mix},m}) \}$$

where $\rho_{\text{mix},m} = M \rho - (m - 1) \rho_{\text{char}} - (M - m) \rho_{\text{vir}}$.

The mass of the volatile material remaining in the grid $(n,m)$ is given by

$$\text{mass}_{\text{vol}} = \frac{\delta x}{M} (\rho_{n,m} - \rho_{\text{char}}) = \frac{\delta x}{M} \min \{ \rho_{\text{vir}} - \rho_{\text{char}}, \max [0,0,(\rho_{\text{mix}} - \rho_{\text{char}})] \}$$

The mass loss rate from grid $(n,m)$ is thus finally determined by

$$m''_{n,m} = \min \{ H_{n,m} / H_{\text{py}}, \text{mass}_{\text{vol}} / \Delta t \}.$$
The overall pyrolysis rate can be obtained by the summation over all the grids and expressed as
\[
m = \sum_{n} \sum_{m} \dot{m}_{n,m} = \sum_{n} \sum_{m} \min(H_{n,m} / H_{py}, \text{mass}_{vol} / \Delta t).
\]  
(87)

The corresponding heat release rate is represented by
\[
\dot{Q} = \dot{m}H_c
\]  
(88)

where \(H_c\) is the heat of combustion.

As a basic test, this thermo-pyrolysis model was used successfully to simulate the Cone Calorimeter tests of both charring material (particle board) and non-charring material (PMMA). An example simulation result is shown in Fig. 13.

This pyrolysis model is very fast and describes the essential physics, in so far as is needed to predict the correct mass loss and heat release rates. It can easily be used in complex cases such as those with a transient incident heat flux and temperature dependent material properties. It is applicable to both charring and non-charring materials and can automatically consider the regression of the surface of the non-charring solid material during its pyrolysis.

Using this pyrolysis model, an ‘equivalent properties’ optimization program can be developed to analyze and fit the Cone Calorimeter test results. A database of the ‘equivalent properties’ of the materials tested in the Cone Calorimeter can thus be created. By using the optimized equivalent properties, this pyrolysis model can be expected to be applicable to realistic composite materials and be used as an alternative to the more complex and expensive models [77].

2.2.2.2 Kinetic-pyrolysis modeling

In a situation where the assumptions in the above thermo-pyrolysis modeling are not applicable, one may need to consider the chemistry directly and relate the mass loss rate with the local solid density and temperature based on the chemical kinetics of pyrolysis. Normally the pyrolysis chemistry can be very complicated and the reaction
path may vary under different external conditions such as the imposed heating and the available oxygen supply. For different fuels, the pyrolysis chemistry can be totally different. For simple solid combustibles such as PMMA, one may assume a first order of pyrolysis reaction and correspondingly express the mass loss rate as a function of density and temperature in an Arrhenius formula. Typically, for such a reaction, one can have

\[ m''' = A(p - p_{\text{char}}) \exp\left(\frac{E_A}{RT}\right) \]  

(89)

where \( A \) is the pre-exponential factor, \( E_A \) is the activation energy, and \( R \) is the universal gas constant.

If more than one reaction is involved in the pyrolysis, one needs to sum up over all the relevant reactions.

For a numerical implementation of the kinetic-pyrolysis modeling, essentially all the numerical methods used in the above thermo-pyrolysis modeling can be used in the same way, including the temperature and density interpolation for the refined grid. With the interpolated local density and temperature for a refined grid \((n,m)\), for a reaction described by eqn (89), the mass loss rate for that refined grid can be simply given by

\[ m'''_{(n,m)} = A(p_{(n,m)} - p_{\text{char}}) \exp\left(\frac{-E_A}{RT_{(n,m)}}\right). \]  

(90)

Using kinetic data measured in [78], this pyrolysis model was applied to simulate a Cone test for particle board and the simulation result was compared in Fig. 14 with results obtained using the thermo-pyrolysis model. The comparison shows that these two models give rather similar results. This indicates that for this case, the very efficient thermo-pyrolysis model is quite valid.

Figure 14: Comparison of results from simulations of a Cone Calorimeter test for a particle board using kinetic and thermo models.
2.2.2.3 Consideration of moisture

For many combustible materials encountered in a conventional fire, such as wood, the internal moisture content can play an important role in the material’s pyrolysis process. Water absorbs a considerable amount of energy during evaporation, and will thus cause some delay in ignition.

For a moisturized solid, when heated, the moisture at a local point may first evaporate and then be convected away to the surrounding. Some water vapor may be transported to the cold part of the solid and then recondense there. The transport of water vapor is heavily dependent on the pressure distribution inside the solid and the permeability of the solid. Typically, the permeability of a solid is highly dependent on the internal structure of the solid and can be inhomogeneous and non-isotropic. To consider all these, a detailed flow dynamic modeling is needed. This can be very complicated. Instead, as a first approximation, one may turn to a simple method.

In a crude approach, the moisture can be described in a way that is similar to the way pyrolysis is described, where one just needs to replace the pyrolysis temperature with water’s boiling temperature, which is 100°C at a pressure of 1.0 atm, and the pyrolysis heat with water’s latent heat.

By assuming 10% of initial moisture, the Cone Calorimeter tests of particle board were re-simulated. Figure 15 gives a typical result which clearly demonstrates the moisture effect.

2.3 Conventional fire simulation cases

Although still under development, CFD fire simulations have been widely used now for different purposes in both research and practical applications. Several fire simulation CFD codes have been developed including KAMELEON [79], SOFIE [80], FDS [81], and SMAFS [82], etc. To briefly illustrate the usage of the conventional fire simulation techniques discussed above, three typical case studies based on these simulation methods will be presented in the following sections. All the simulations discussed in this chapter were performed using the software package SMAFS [82] developed by the author.

![Figure 15: Moisture effect in a simulation of a Cone Calorimeter test for a particle board (a kinetic pyrolysis model was used).](image-url)
2.3.1 CFD simulation of flame spread in room corner fire

This case study comes from an early attempt made to simulate the flame spread in room corner fires, in both 1/3 and full scale scenarios. This simulation was a comprehensive study based on the RANS concept, in which essentially all the main physical sub-processes mentioned above were considered.

In this case study, the gas temperature, solid temperature, heat release history, and char layer development are all analyzed and compared with experimental measurement. The simulation results are rather promising. The predicted flame spread pattern and heat release history in the 1/3 scale scenario are shown and compared with experimental measurements in Figs 16 and 17. (In Fig. 17, the total heat release includes the energy released from combustion inside the room and the energy associated with the fuel which leaves the room unburnt. This unburnt fuel may burn outside the room.) The details of this study are presented in [60].

Figure 16: Flame spread pattern in the 1/3 scale scenario, indicated by surface temperature (in kelvin) \(t = 300\) s, threshold = 600 K.

Figure 17: Calculated and measured heat release rates in the 1/3 scale scenario. The symbol (c) denotes using Cone data input method and (p) the pyrolysis model [60] (©Elsevier Science Ltd., with permission).
2.3.2 CFD simulation of complex practical fire

This is another RANS simulation of fire and flame spread. Unlike the previous case which is mainly for research development and validation, this case study deals with a practical real life fire which happened in Gothenburg, Sweden, in 1998. This fire caused big losses in both of property and people’s life. Figure 18 shows an overview of the building.

A fire was started in a half-flight of stairs in the emergency exit stairwell while the door on the ground floor was left partially open. After a short while, through the emergency exit door, the fire quickly spread into the dance hall from the stairwell. Due to the strong heating, some combustible in the dance hall was ignited and the fire became more severe.

After the fire, an extensive investigation including this CFD simulation was organized by the Swedish Board of Accident Investigation and the police, to gather necessary information for the perception and interpretation of events, actions taken as well as the evacuation process.

Due to its complexity and high demand in CPU time, this computation was performed in parallel on a SGI 2000 machine using a parallel algorithm presented in [74]. The results of this CFD simulation correspond with the real fire pattern very well and help explain observed fire phenomena. Figure 19 shows typical plots of heat flux and window flame temperature. The details of this simulation can be found in [83].

Figure 18: Different views of the building [74] (©Taylor & Francis).
2.3.3 LES of a turbulent buoyant diffusion flame

This case study presents a LES of non-premixed turbulent combustion in a pool fire. The sub-grid stresses were modeled using the Smagorinsky model. The SGS scalar fluxes in the filtered scalar transport equations were modeled based on simple gradient transport hypothesis with assumed constant SGS Prandtl/Schmidt numbers. The SGS randomness of the turbulent combustion was taken into account based on a flamelet concept with a prescribed SGS probability density function. With the nucleation, surface growth, coagulation, and oxidation considered, sooting was modeled using a flamelet-based soot model where the balance equations for soot mass fraction and soot number density are solved. The instantaneous thermal radiation was calculated using the discrete transfer method with the radiation property of the participating medium evaluated by an approximated FASTNB model. The details of the models have already been discussed in previous sections.

The configuration of the problem is simple. Fuel (propane) was injected into an open environment from a square burner located at the bottom center of the domain. The size of the whole computation domain was 0.475 m \((x) \times 1.25\) m \((y), \text{vertical direction}) \times 0.475\) m \((z)\).

A non-uniform grid of 96 \times 128 \times 96 was used in the computation, with clustering applied to the flame zone to provide an optimum resolution. Figure 20 presents a short sequence of the instantaneous temperature profile from LES showing a buoyant flame’s puffing.

3 CFD simulation of spontaneous ignition in porous fuel storage

This section presents the recently developed CFD simulation techniques for prediction of spontaneous ignition in porous fuel storage.

Unlike the already discussed conventional fires, spontaneous combustion in porous fuel storage (including bio-fuel storage and other fuel storage such as coal storage) is mainly due to heat generation by low temperature oxidation and bio-activity. When the generated heat cannot be adequately dissipated into the surrounding environment, the temperature rises and in turn further speeds up the exothermic oxidation process to eventually result in a self-ignition. Spontaneous ignition of fuel storage is a complicated problem which is dependent on many physical and chemical processes. The processes involved mainly include fluid flow, heat transfer, mass transfer, water condensation and evaporation, bio-activity, and chemical reactions, etc. Because of the large
number of involved processes, spontaneous ignition relies on many different parameters which may affect the involved processes. Some well-known typical parameters which have an important influence on spontaneous ignition are storage size, moisture content, permeability, porosity, fuel particle size, and fuel’s low temperature reactivity. Environmental conditions such as the ambient temperature and wind flow also have determining effects on spontaneous ignition.

Spontaneous ignition of a porous fuel storage is of great importance in the fuel industry and poses a serious safety and economic problem which can harm the environment and cause big economic losses. Due to economic and safety concerns, it is of great interest to investigate how these parameters and conditions can affect spontaneous ignition and thus to find out under which conditions the spontaneous ignition can occur or be avoided.

Because of its practical importance, much experimental and theoretical effort [84–91] has been devoted to this area. Among the theoretical analysis, the most notable pioneer work is the well-known classical Frank-Kamenetskii theory [84]. In the classical Frank-Kamenetskii analysis, in order to obtain an analytical solution on such a complicated problem, heavy simplifications are made in many aspects regarding the heat and mass transfer, chemical reaction, geometry, and boundary conditions. The advantage of the classical Frank-Kamenetskii analysis is that it explicitly gives the representative relations between some important parameters controlling the spontaneous ignition. Unfortunately, these assumptions are highly invalid in many practical situations.
This seriously limits the applicability of the Frank-Kamenetskii analysis. CFD modeling is a good strategy to abandon assumptions which are purely imposed by the difficulty of obtaining a mathematical solution of the differential equations and thus improve the applicability of the theoretical analysis. CFD numerical modeling has the possibility to solve a set of coupled partial differential equations and thus offers great advantage of high flexibility to simultaneously take into account different coupled processes. In the numerical modeling, the assumption and simplification can be limited to the aspects of the physical understanding.

3.1 The comprehensive spontaneous ignition CFD model

Self-ignition in a porous fuel storage such as biomass fuel or coal storage is fully dependent on the competition between heat generation inside the fuel storage and its heat loss to the environment. Normally, in a biomass fuel storage, heat can be generated due to bioactivity which can play a major role when temperature is less than about 350 K and chemical reaction which becomes dominant as temperature increases. Usually, the bio-activity is also heavily dependent on local moisture content and oxygen concentration. The exothermic chemical reaction is largely proportional to the local oxygen concentration. The local moisture content and oxygen concentration are governed by mass transport. For moisture, the condensation and evaporation can also be critically important. On the other hand, for heat loss, the heat transfer inside the fuel storage and the heat exchange between the fuel storage and its environment are governed by radiation, convection, and diffusion.

In order to perform a theoretical study of self-ignition in a porous fuel storage, consideration must be given to all the important governing processes. In a CFD modeling, a set of coupled governing partial differential equations are solved to obtain the storage’s state evolution.

The governing equations, which include the continuity equation, momentum equation, mass transport equation, and energy equations for both gas and solid phases, are listed below.

Continuity equation
\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = S_{\text{gas}}
\]

Momentum equation
\[
\varphi \frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \varphi^2 \left\{- \frac{\partial \rho}{\partial x_i} - \frac{\mu}{\kappa} u_i + \frac{\partial}{\varphi \partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} \right) - \frac{c_F \rho_g}{k^{0.5}} (u_i u_j)^{0.5} u_j + \rho_s a_{gi} \right] \right\}
\]

Mass conservation equation for chemical species
\[
\varphi \frac{\partial \rho_s Y_i}{\partial t} + \frac{\partial (\rho_s Y_i u_j)}{\partial x_j} = \varphi \frac{\partial}{\partial x_j} \left[ \frac{\mu}{S_c} \frac{\partial Y_i}{\partial x_j} \right] + S_{Y_i}
\]

Energy conservation equation for gas phase
\[
\varphi \frac{\partial \rho_s H_g}{\partial t} + \frac{\partial (\rho_s H_g u_j)}{\partial x_j} = \varphi \frac{\partial}{\partial x_j} \left[ \frac{\mu}{P_r} \frac{\partial H_g}{\partial x_j} \right] + S_{H_g}
\]
Energy conservation equation for solid phase

\[
\frac{\partial \rho_s H_s}{\partial t} = \frac{\partial}{\partial x_j} \left[ \lambda_s \frac{\partial H_s}{\partial x_j} \right] + S_{H_s} \tag{95}
\]

The moisture balance in solid phase

\[-\rho_s \frac{\partial W}{\partial t} = r_w \tag{96}\]

In the above equations, \(\varphi\) is the porosity, \(\kappa\) is the permeability, \(c_F\) is the form-drag constant.

In order to close the above equations, the source terms must be given based on the solved variables. The details of these source terms are omitted here and can be found in [92].

### 3.2 CFD simulation of spontaneous ignition experiment

The spontaneous ignition experiments simulated are basket heating tests. The biomass fuels used include wood sawdust, and wood pellets of 6 mm in diameter. The main equipment used was a temperature-controlled oven of 0.34 m (depth) \(\times\) 0.40 m (height) \(\times\) 0.40 m (width) with recirculating air. A stainless-steel 0.6 mm mesh basket filled with solid fuel was suspended in the oven. The size of the basket is 0.1 m \(\times\) 0.1 m \(\times\) 0.1 m. In order to trigger and speedup the spontaneous ignition process, the oven was heated up and maintained to have a temperature of 180°C for the sawdust case and 200°C for the wood pellets case. The temperature evolution inside the basket was monitored using five 0.25 mm type K thermocouples which were placed between the volume center of the basket and center of the basket at one side surface.

The basket tests were simulated using SMAFS [82]. Figure 21 shows the comparison between predicted and measured temperature histories for the five locations of the sawdust case. The level-off phenomenon in the temperature history is due to moisture effects. At about 250 min, the temperature curves cross each other. This indicates a high potential of spontaneous ignition.

As can be seen in Fig. 21, the prediction reproduces the experimental measurements very well. The temperature rise pattern, the ‘level-off’ temperature and temperature crossing time and values are all well-predicted. This indicates that all the important processes were well-captured by

![Figure 21: Predicted and measured temperature histories at five locations (©IAFSS).](image-url)
the numerical simulation. To provide a better data comparison, the predicted temperature evolution is compared with measurement for each individual point. Figure 22 gives an example comparison for point 3.

To have an overview of the spatial distribution of the important moisture content, a typical visualization of moisture content at a time of 120 min is presented in Fig. 23 showing a heart pattern distribution.

As indicated earlier, the solid fuel of 6 mm wood pellets was also studied. The results are similar with those for sawdust and good agreement between prediction and measurement is also obtained. More details of this simulation can be found in [93].

4 Conclusions

This chapter presents a review of CFD simulations of both conventional fires and spontaneous ignition in a porous fuel storage. For conventional fire simulations, the discussion is focused on
modeling of different essential sub-processes in fires including turbulence, turbulent combustion, thermal radiation, soot formation, heat transfer inside solids, and pyrolysis of combustible solid fuel, etc. For simulations of spontaneous ignition in a porous fuel storage, some interesting recent developments are presented.

References


