

AND LAMINAR SMOKE POINT SOOT MODEL TO THE

LARGE EDDY SIMULATION OF FIRE DYNAMICS

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FOR REFERENCE ONLY

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ABSTRACT

The original turbulent energy cascade of eddy dissipation concept (EDC) has been extended to the LES framework, assuming that there is always a structure level on which the typical length scale is equivalent to the filter width of large eddy simulation (LES). The velocity scale on this structure level could be calculated from the sub-grid scale (SGS) kinetic energy, provided that this kinetic energy transport equation is solved in LES. All other quantities would thus be calculated on this structure level according to the general formulations from the original turbulent energy cascade. Based on this known structure level, the total kinetic energy and dissipation rate could be estimated with the integral length scale being assumed to be equivalent to the characteristic length of fire plume. Consequently, the Kolmogorov time scale and the integral time scale could also be calculated and then applied in the soot model development.

The laminar based smoke point soot model (SPSM) is also extended to the LES framework. The filtered soot mass fraction transport equation is solved with the thermophoresis term neglected. The filtered soot formation rate is treated using the concept of partially stirred reactor (PaSR). This rate is thus associated with the laminar based soot formation rate substituted with the filtered properties through the expression of κ . Note that in κ the soot formation chemical time scale is assumed to be proportional to the laminar smoke point height (SPH) while its turbulent mixing time is supposed to be the geometric mean of the Kolmogorov time scale and integral time scale. Furthermore, a new soot oxidation model is developed by imitating the gas phase combustion model, i.e. EDC, as the soot particles are assumed to be the solid phase of the fuel. Note that the turbulent mixing time scale for soot oxidation has been chosen to be the same as soot formation. The soot formation and oxidation models are coupled to treat the effect of soot on the fuel distribution and energy transport.

The approaches to calculate flame height, radiative fraction, and surface emissive power (SEP) have also been developed for sooty flames. The models and approaches mentioned above are implemented into FireFOAM, which is a fully compressible solver based on the platform of OpenFOAM. A series of fire scenarios, involved with different fuels including methanol, methane, heptane and toluene, and with different scales ranging from 30 cm to 56 m, are performed for validation studies. The detailed comparisons, such as mean velocity and its fluctuation, mean temperature and its fluctuation, soot volume fraction and its fluctuation, turbulent heat flux, time scales and length scales, flame height, radiative fraction, SEP and so on, between predictions and measurements demonstrate the capability of the current models. This thesis is dedicated to my wife Feiyang Liu, and my parents Binggong Chen and Faying Liu. Their infinite love makes me feel they are always with me, although we are so far away! They are my everything!

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LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamics
СМС	Conditional Momentum Closure
D	Diameter
DNS	Direct Numerical Simulation
DOM	Discrete Ordinate Method
DRM	Discrete Reaction Model
DTM	Discrete Transfer Method
EBU	Eddy Break-Up
EDC	Eddy Dissipation Concept
FDS	Fire Dynamics Simulator
FVM	Finite Volume Method
Н	Height
HRR	Heat Release Rate
LES	Large Eddy Simulation
LNG	Liquefied Natural Gas
NAR	Narrow Angle Radiometer
NIST	National Institute of Standards and Technology
РАН	Polycyclic Aromatic Hydrocarbon
PaSR	Partially Stirred Reactor
PDF	Probability Density Function
PISO	Pressure Implicit with Splitting of Operator
RANS	Reynolds-Averaged Navier-Stokes
RHS	Right Hand Side

RMS	Root Mean Square
RTE	Radiative Transfer Equation
SEP	Surface Emissive Power
SFM	Solid Flame Model
SGS	Sub-grid Scale
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
SPH	Smoke Point Height
SPSM	Smoke Point Soot Model
WAR	Wide Angle Radiometer

Chapter 1

Introduction

1.1 BACKGROUND

Fire hazard, causing human death and property damage, is a very big threat to our society. It is reported in [1] that in the lifetime of a person in US, about 1 in 800 will die by fire, and the economical loss due to fires is estimated to be 0.81 % of the annual GDP for most developed countries. In China, the number of fire incidents in 2011 is reported as 125,402 with the fire deaths of 1106 and the direct economical loss of 1.88 billion Yuan [2]. Therefore, it is very important to understand the fundamentals of fire phenomena, and to reduce the fire related losses.

There are mainly two approaches to study the fire dynamics. One approach is conducting fire tests, including full scale fire tests and reduced scale fire tests. One could observe fire behaviours directly from experiments, measure important quantities, and then evaluate the potential threats. So far a lot of experimental studies have been performed in the fire community, and indeed those efforts have made great contributions to the fire science. However, sometimes experimental work is costly, particularly the full scale real fire tests.

The other approach is performing numerical simulations, based on the solution of relevant governing equations. This has become more and more popular with the development of computer science and technology. This

approach is believed to be more cost effective than the experimental approach. For example, we could easily change the initial and boundary conditions in the numerical work. However, this approach is not as reliable as experiments at present, as its performance depends on the quality of the numerical models and competence of the investigator. Hence, there is still some argument about the role of numerical simulations in fire research. Although numerical simulations could not totally replace experiments at present, they can help us gain a better insight into fire dynamics.

This thesis focuses on numerical simulations of fire dynamics. Fire dynamics is characterized by the complex interaction of several major physical processes including buoyancy-driven flow, turbulence, non-premixed combustion, soot production as well as radiative heat transfer. Models are needed to better account for these physical processes, as at present we cannot afford to solve the governing equations similarly like direct numerical simulation (DNS) in most fire scenarios. The aim of this thesis is to develop a robust model for the consideration of gas phase combustion and of soot production in fires, in the framework of large eddy simulation (LES) which is becoming increasingly popular.

1.2 OUTLINE OF THE THESIS

In Chapter 2, the original eddy dissipation concept (EDC) combustion model will be extended from Reynolds-averaged Navier-Stokes (RANS) to the LES framework, according to the turbulent energy cascade from the large eddies down to the small eddies. The turbulent scales, such as integral time scale and Kolmogorov time scale, would be calculated based on this extension, which are important quantities to characterize the gas phase combustion, soot formation, and oxidation. Moreover, a new formula will be developed for the reacting fraction of fine structures in EDC, in order to tackle some problems due to the original expression. A formula for the mass fraction of fine structures will also be modified.

In Chapter 3, a laminar smoke point soot model (SPSM) will be extended to the LES framework. Soot formation is accounted for by using the partially stirred reactor (PaSR), in which the turbulent mixing time scale is assumed to be the geometric mean of integral time scale and Kolmogorov time scale, both calculated from the newly developed EDC. Moreover, the chemical soot formation time scale will be assumed to be proportional to the laminar smoke point height. A new soot oxidation model will be developed, as the original predescribed constant or profile would give rise to non-physical soot volume fraction distributions, as well as the numerical instability.

In Chapter 4, the radiation model will be described, with the finite volume method (FVM) being used to discretize the radiative transfer equations (RTE). Optically thin assumption is adopted for the optically thin flames, such as methanol and methane fires, and therefore the incident radiation will be neglected to avoid the resolution of RTE on the spectral bands. For other flames, the grey body assumption will be employed, and the essential total absorption coefficient, including gas absorption coefficient and soot absorption coefficient, need to be determined. Three different methods to calculate the surface emissive power (SEP) will be described.

In Chapter 5, the governing equations for mass, momentum, gas species, soot and sensible enthalpy will be presented, in particular the treatment of the

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soot effect on the energy and fuel distribution. Special treatment of pressure will be considered for the fire scenarios in the cross wind. The approaches to determine the flame height, radiative fraction and flame tilted angle will also be described in this chapter as well as the cross wind inlet boundary condition.

In Chapter 6, detailed results and discussions will be presented for a series of small/medium scale methanol, methane, heptane, and toluene fires. Not only the traditional properties, such as temperature, velocity, and soot volume fraction, but also the turbulent quantities, like fluctuations, integral scales, dissipation rate and kinetic energy, will be analyzed in order to understand thoroughly the capability of those new developed models.

In Chapter 7, detailed results and discussions will be performed for a series of large scale LNG pool fires, aiming to investigate the potential of those models. Heat release rate, flame height, flame tilted angle, radiative fraction and SEP will be examined by comparing with the relevant experimental data.

In Chapter 8, we will conclude the thesis, and also provide recommendations for future work.

Chapter 2

Combustion Model

2.1 INTRODUCTION

Fire modeling using computational fluid dynamics (CFD) techniques has been evolving for decades. Various models have been proposed for the underlying combustion chemistry. However, due to the assumptions made during the development of the model, there still lacks a universal model that is suitable for all combustion scenarios in different combustion systems and fires.

In the fire community, the mixture fraction based combustion model is widely used by assuming the Shvab-Zel'dovich formulation [3, 4], irreversible and infinitely fast chemistry and the Burke-Schumann flame structure [3, 4]. The probability density function (PDF) approach is often adopted to take into account the effect of turbulence on combustion. Reasonably good agreement [5] of important quantities such as temperature and velocity has been achieved according to comparison with experimental data. However, this model cannot deal with the effect of soot on fuel distributions and on energy transport, which is the aim of this current study. Moreover, this model cannot provide the framework to further consider fire behaviors under the water spray system, which is a big concern for our sponsor, i.e. FM Global.

Magnussen and Hjertager [6] proposed the first version of the EDC based on the eddy-break-up (EBU) model of Spalding [7, 8], assuming that the

chemical reaction rate is controlled by the mixing rate of fuel and oxidizer instead of the mixing rate of unburned and burned gas in the EBU. In this version, the constant is calculated either by the collision mixing model [6] or by the viscous mixing model [9]. Bilger [10] suggested that the coefficient is dependent on the PDF of the mixture fraction, and one can use the mixture fraction and its deviation to calculate it [11]. Bilger's work demonstrated that its value is not strongly dependent on the shape of PDF and its average value across the flame is close to that calculated by the collision mixing model [12]. However, the average value is likely to produce large errors at the fuel side where more accurate computational procedure is desirable. Subsequently, Magnussen [13] incorporated the significance of fine structures into EDC. Chemical reactions are assumed to take place in these fine structures and the extended model is formulated in a way that both finite rate chemistry and fast chemistry can be used. Magnussen [14] gave a comprehensive review of the various modified version of the EDC model and demonstrated its improved predictions on some test cases. However, there still exist some limitations about the treatment of the reacting fraction within the fine structures, which is addressed in the present study.

The EDC model was widely used in fire applications. Cox [15] applied JASMINE to model enclosure fires with forced and natural ventilation using the EDC for validation and achieved reasonably good agreement with experimental data. Hutanen [16] performed fire simulations in a turbine hall using the PHOENICS code. Adiga [17] simulated a 0.25 m 28 kW turbulent methane fire and found that the centerline properties such as mean temperature, axial velocity and entrainment behaviors are generally well reproduced by the EDC. Wang [18] presented results on steady-state turbulent burning along a vertical rectangular channel in which a buoyancy-induced draft develops. The predictions of temperature, velocity and turbulent quantities were in good agreement with the experimental data. Novozhilov [19] tracked fire spread of solid materials and simulated the extinguishment by water sprays. The predictions agreed well with the experiment findings. Yoon [20] carried out the studies on fire extinction behavior using the EDC-based model [21] developed at Sandia National Laboratories. His predictions were qualitatively encouraging.

However, all the above studies were carried out in the RANS context. Although the effect of turbulence on the combustion process is taken into account, the well known limitations of the turbulence models in RANS have to some extent limited the accuracy of these predictions. Since the EDC is highly dependent on the accuracy of the predictions for fuel-air mixing, for which the LES approach is deemed to be more appropriate, its extension to the LES context should render the model more suitable to capture the fine details of the combustion process. More recently, Panjwani [22] attempted the extension of the EDC to LES and numerical instability was reported. The validation study for a turbulent piloted non-premixed methane/air jet flame (Sandia Flame D) suggested that the model constant had to be changed from 1.01 to 0.25. The requirement of such ad-hoc adjustment for model constant poses difficulties for it to be applied to other scenarios where experimental data is not available. In a more robust approach, the constant should be computed dynamically rather than artificially specified.

In this Chapter, the EDC combustion model will be extended from RANS to the LES framework, according to the turbulent energy cascade. Moreover, a new formula will be developed for the reacting fraction of fine structures in EDC,

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in order to tackle the lifted problem due to the original expression. The original expression for the mass fraction of fine structures will be also modified.

2.2 EDDY DISSIPATION CONCEPT

The detailed description of original EDC is elaborated in Ref. [14], based on RANS. Here the RANS-based EDC will be extended to the LES framework through the turbulent energy cascade. Furthermore, the typical time scales including Kolmogorov time scale and integral time scale will be achieved, which are important for the soot development in the next Chapter.

2.2.1 Turbulent Energy Cascade

A stepwise turbulent energy cascade [13] is supposed to take place from mean flow down to Kolmogorov scale, and the heat generation resulting from the dissipation of turbulence energy is assumed to mainly occur on the small scales where production and dissipation balance. This assumption is believed to be independent of the chosen turbulence models, either RANS or LES. Given the fact that the filter width of LES generally falls between the Kolmogorov and integral length scale, we assume that there is a structure level for the presence of SGS properties, such as SGS kinetic energy and filter width Δ , in the stepwise turbulent cascade, as shown in Fig. 2.1. As properties on this ' Δ ' level can be determined directly from a SGS turbulence model, we should then be able to derive characteristic variables on other levels. The total kinetic energy and its dissipation rate may also be calculated from parameters on this known structure level and then described with SGS quantities.



Fig. 2.1 The stepwise turbulent energy cascade in the LES framework

In Fig. 2.1, u_n , L_n and ω_n represent the velocity scale, length scale and strain rate on the *n*-th structure level respectively. Following Ertesvåg and Magnussen [13], the strain rate ω_n is assumed to be equal to $2\omega_{n-1}$ with regard to the relationship between two adjacent structure levels. q_n represents thermal energy resulting from dissipation on each level while W_n stands for the sum of mechanical energy on all subsequent levels. On the *n*-th level, W_n and q_n may be expressed as [13]

$$W_{*} = \frac{3}{2} C_{D1} \omega_{*} u_{*}^{2}$$
(2.1)

$$q_n = C_{D2} \upsilon \omega_n^2 \tag{2.2}$$

$$\omega_n = \frac{u_n}{L_n} \tag{2.3}$$

$$\omega_n = 2\omega_{n-1} \tag{2.4}$$

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where v is the molecular kinematic viscosity, C_{D1} and C_{D2} are model coefficients. According to Eqs. (2.2) and (2.4),

$$q_n = 4q_{n-1} \tag{2.5}$$

The total dissipation rate of kinetic energy may be modeled as [13]

$$\varepsilon = q' + q'' + \dots + q_n + q_{n+1} + \dots + q_{SGS} + q_1 + \dots + q'$$
 (2.6)

Substituting Eq. (2.5) into Eq. (2.6) and then applying series theory,

$$4q^{*}-q'=3\varepsilon \tag{2.7}$$

Similarly, W_{scs} on the ' Δ ' level may be expressed as

$$W_{scs} = q_{scs} + q_1 + q_2 + \dots + q^*$$
 (2.8)

Substituting Eq. (2.5) into Eq. (2.8),

$$4q^* - q_{SCS} = 3W_{SCS} \tag{2.9}$$

Subtracting Eq. (2.9) from Eq. (2.7),

$$\varepsilon = W_{SGS} + \frac{1}{3}q_{SGS} - \frac{1}{3}q'$$
 (2.10)

q' is believed to be negligible since the dissipation into heat mainly takes place on the small scales rather than the integral scale. According to Eqs. (2.1)-(2.3), Eq. (2.10) could be rewritten as

$$\varepsilon \approx W_{SGS} + \frac{1}{3}q_{SGS} = \frac{3}{2}C_{D1}\frac{u_{SGS}^{3}}{\Delta} + \frac{1}{3}C_{D2}\nu\frac{u_{SGS}^{2}}{\Delta^{2}}$$
(2.11)

 u_{scs} is estimated to be $\sqrt{\frac{2}{3}k_{scs}}$, where k_{scs} is SGS kinetic energy obtained from a LES model such as sub-grid kinetic energy model [23]. Therefore,

$$\varepsilon \approx \sqrt{\frac{2}{3}} C_{D1} \frac{k_{SGS}^{\gamma_2}}{\Delta} + \frac{2}{9} C_{D2} \upsilon \frac{k_{SGS}}{\Delta^2}$$
(2.12)

Based on the energy conservation on all the structure levels,

$$W' = \varepsilon = \frac{3}{2} C_{D1} \frac{(u')^3}{L'}$$
 (2.13)

where L' is the integral length scale. u' is calculated from $\sqrt{\frac{2}{3}k}$, and k is the

total kinetic energy. Note that Eq. (2.13) could be also converted to

$$k = \left(\frac{3}{2C_{D1}^{2}}\right)^{1/3} \left(\varepsilon L'\right)^{2/3}$$
(2.14)

For the last structure level, W^* is expected to be equal to q^* in terms of the energy conservation. Combining with Eq. (2.7), the characteristic length and velocity scale on the last level could be described as

$$L^{*} = \frac{2}{3} \left(\frac{3C_{D2}}{C_{D1}}^{3} \right)^{1/4} \left(\frac{\upsilon^{3}}{\varepsilon} \right)^{1/4}$$
(2.15)

$$u^{*} = \left(\frac{C_{D2}}{3C_{D1}^{2}}\right)^{V4} (\upsilon \varepsilon)^{V4}$$
(2.16)

In this study, these two scales are assumed to be the Kolmogorov length and velocity scale [24], respectively, implying $C_{D1} = 0.5$ and $C_{D2} = 0.75$. Turbulent mixing time scales, such as Kolmogorov time scale (τ_n) and integral time scale (τ_l), are calculated from:

$$\tau_{\eta} = \left(\frac{\nu}{\varepsilon}\right)^{\nu_2} \tag{2.17}$$

$$\tau_{i} = \frac{k}{\varepsilon} \tag{2.18}$$

2.2.2 Reaction Rate

Chemical reactions are assumed to take place only in the fine structures, i.e. the last structure level of the turbulent energy cascade; and each of them is regarded as a well stirred reactor [9]. Subsequently, the remaining reactants and newly formed products may mix with the surrounding fluids. In fires, the chemical reaction time scale is generally less than the turbulent mixing time scale. Thus the reaction rate is likely to be controlled by turbulent mixing. In this study, the fast chemistry with Burke-Schumann flame structure [3] is assumed for the combustion, and hence the filtered reaction rate of each species ($\bar{\omega}_{m,r}$) for the gas phase combustion can be written as [9]

$$\overline{\omega}_{m,g} = \left(v_m'' - v_m'\right) \frac{MW_m}{MW_{fu}} \overline{\omega}_{fu}$$
(2.19)

$$\overline{\omega}_{h} = C_{EDC} \overline{\rho} \dot{m} \, \min\left(\tilde{Y}_{h}, \frac{\tilde{Y}_{O_{c}}}{s}\right)$$
(2.20)

$$C_{EDC} = \frac{\gamma \chi}{1 - \gamma \chi} \tag{2.21}$$

where v_i'' and v_i' are the molar stoichiometric coefficients of each species in the global single-step kinetics, MW_i is the molar weight of each species, $\overline{\rho}$ is the filtered density, \tilde{Y}_i is the density-weighted species mass fraction, s is the stoichiometric oxygen-fuel ratio, and subscripts fu and O_2 refer to fuel and oxygen, respectively. Note that γ and χ will be considered in the following subsection. The mass transfer rate (m^*) between the fine structures and surrounding fluids could be calculated from [13]

$$\dot{m}^{*} = \frac{2u^{*}}{L^{*}} = \left(\frac{3}{C_{D2}}\right)^{1/2} \left(\frac{\varepsilon}{\upsilon}\right)^{1/2}$$
(2.22)

2.2.2.1 Mass Fraction of Fine Structures

The mass fraction of fine structures (γ) might be related to the turbulence intermittency [13]. It is written as below in the early version of EDC [13]:

$$\gamma \approx \frac{L^{*}}{L^{\prime}}$$
(2.23)

Later, it is expressed as [14]

$$\gamma \approx \left(\frac{L}{L'}\right)^{2/3} \tag{2.24}$$

Note that Eq. (2.23) is quite similar to the model by Corrsin [25], and he suggested that the small-scale fine structures consisted of vortex sheets. Later, Tennekes [26] proposed that the fine structures were in the shape of vortex tube, and γ would be expressed as

$$\gamma \approx \left(\frac{L^2}{\lambda}\right)^2 \tag{2.25}$$

where λ is the Taylor micro scale, defined as

$$\lambda = \sqrt{\frac{10\nu k}{\varepsilon}}$$
(2.26)

Frisch et al [27] suggested this fraction as

$$\gamma = \left(\frac{L}{L'}\right)^{3-D} \tag{2.27}$$

The constant D was assumed to be 2.5, theoretically representing the shape of fine structures, while Lesieur [28] suggested a value closer to 3, based on experimental data.

In this study, Eq. (2.27) is adopted, and D is set as 2.8 following the turbulence structure analysis [29]. Now the key issue would be how to obtain this integral length scale L'. Actually, the integral length scale is also vital for the calculation of total kinetic energy k, as well as the integral time scale τ_i . In RANS, the total kinetic energy k and total dissipation rate ε are generally computed from their own transport equation. Thus, one could estimate L' through Eq. (2.14), and so could τ_i based on Eq. (2.18). However, in LES only SGS kinetic energy k_{scs} transport equation could be solved. As ε can be estimated from Eq. (2.12), there would be two unknowns in Eq. (2.14), either k or L'. Mathematically one of them needs to be specified in order to find another one. Apparently, it is impossible to give the value of k directly, and L' should thus be pre-described. It is known that the integral length scale is often associated with the geometric characteristic of a given system [3]. In fires, this scale is likely to be proportional to the characteristic length of fire plume [30] expressed as

$$L' = \left(\frac{Q}{\rho_x c_p T_x \sqrt{g}}\right)^{2/3}$$
(2.28)

where Q is the heat release rate, kW. Eq. (2.28) is used to approximate k and τ_i in this study.

In our previous work [31], the problem of γ was temporarily tackled by assuming it as a constant. Substituting Eq. (2.14) and Eq. (2.15), Eq. (2.27) would be recast as

$$\gamma = \left(\frac{4C_{D2}}{3C_{D1}}^{3}\right)^{(3-D)/4} \left(\frac{\upsilon\varepsilon}{k^{2}}\right)^{(9-3D)/4}$$
(2.29)

If both the total kinetic energy k and total dissipation rate ε are replaced with their SGS quantities, following the study by Panjwani [22], Eq. (2.29) would become

$$\gamma = \left(\frac{4C_{D2}^{3}}{3C_{D1}^{6}}\right)^{(3-D)/4} \left(\frac{\upsilon \varepsilon_{SGS}}{k_{SGS}^{2}}\right)^{(9-3D)/4}$$
(2.30)

By substituting Eq. (5.13) and Eq. (5.14), Eq. (2.30) could be transformed to

$$\gamma = \left(\frac{4C_{D2}}{3C_{D1}}\right)^{(3-D)/4} \left(C_k C_k\right)^{(9-3D)/4} \left(\frac{\upsilon}{\upsilon_i}\right)^{(9-3D)/4}$$
(2.31)

In the LES framework, turbulent viscosity v_i might become zero due to the local laminarization during combustion [22], causing γ , the mass fraction occupied by the fine structures (physically ranging from 0 to 1) to be ill-defined, and the EDC has no meaning for such large values of γ . In consideration of this, an upper limit of γ is set as 1 in Ref. [22]. Eq. (2.31) can be further simplified as follows with the assumption of $v = v_i$:

$$\gamma = \left(\frac{4C_{D2}}{3C_{D1}}\right)^{(3-D)/4} (C_{t}C_{s})^{(9-3D)/4}$$
(2.32)

Now γ becomes a constant, implying that mass fraction occupied by fine structures is fixed once the LES model coefficients, including C_t and C_c , are specified before simulations. The starting point is that C_{EDC} in Eq. (2.20) is prescribed as a constant in the early version of EDC [6, 11]. In addition, this simple treatment is supposed to tackle the numerical instability in the wall region reported in Ref. [22]. However, this approach couldn't help us to achieve the integral time scale τ_l , which is employed to account for the soot model development. Actually, the inclusion of Eq. (2.28) would be regarded as the
extension of our early work [31], and this inclusion would be the default approach in this study.

2.2.2.2 Reacting Fraction of Fine Structures

The original expression of χ is written as [14]

$$\chi = \frac{\frac{\tilde{Y}_{pr}}{(1+s)}}{\min\left(\tilde{Y}_{fu}, \frac{\tilde{Y}_{o_2}}{s}\right) + \frac{\tilde{Y}_{pr}}{(1+s)}}$$
(2.33)

where \tilde{Y}_{pr} is the density-weighted mass fraction of products, expressed as

$$\tilde{Y}_{pr} = 1 - \tilde{Y}_{fr} - \tilde{Y}_{O_2} - \tilde{Y}_{N_2}$$
(2.34)

Using this original expression, the flame would be lifted from the pool, which is believed to be non-physical for pool fires. This issue would be elaborated in details in Chapter 6. Thus, a new formulation of χ is proposed here.

Given a mixture of fuel and oxidizer at the location where the temperature is higher, the possibility of combustion taking place near this area should be larger. Therefore, it is possible to assume χ is proportional to the flame temperature of the mixture, written as

$$\chi = CT \tag{2.35}$$

In this study, τ in Eq. (2.35) is assumed to be the adiabatic flame temperature, and extinction effect and radiation loss are thus not taken into consideration. Under the assumption of Shvab-Zel'dovich formulation [3, 4], irreversible and infinitely fast chemistry and of the Burke-Schumann flame structure [3, 4], the adiabatic flame temperature is only a linear function of the mixture fraction z as shown in Fig. 2.1.



Fig. 2.1 Relationship between mixture fraction and adiabatic flame temperature Therefore, if $0 \le Z < Z_{y}$,

$$\frac{T - T_0}{T_{\max} - T_0} = \frac{Z}{Z_{st}}$$
(2.36)

and if $Z_{st} \leq Z \leq 1$,

$$\frac{T - T_f}{T_{\text{max}} - T_f} = \frac{1 - Z}{1 - Z_{y}}$$
(2.37)

where T_{max} is the maximum adiabatic flame temperature, and T_0 and T_f are ambient temperature in oxygen and fuel stream, respectively. Recasting Eq. (2.36) and Eq. (2.37),

$$T = \begin{cases} \frac{Z}{Z_{st}} (T_{\max} - T_0) + T_0, & \text{if } 0 \le Z < Z_{st} \\ \frac{1 - Z}{1 - Z_{st}} (T_{\max} - T_f) + T_f, & \text{if } Z_{st} \le Z \le 1 \end{cases}$$
(2.38)

Substituting Eq. (2.35) into Eq. (2.38),

$$\chi = \begin{cases} C\left(\frac{Z}{Z_{it}}(T_{\max} - T_0) + T_0\right), & \text{if } 0 \le Z < Z_{it} \\ C\left(\frac{1 - Z}{1 - Z_{it}}(T_{\max} - T_f) + T_f\right), & \text{if } Z_{it} \le Z \le 1 \end{cases}$$
(2.39)

Since theoretically complete combustion takes place at the location where $Z = Z_{sr}$, it is possible to assume the reacting fraction of fine structures achieves its maximum value there, i.e. $\chi = 1$. Combining with Eq. (2.39),

$$C = \frac{1}{T_{\max}} \tag{2.40}$$

Thus,

$$\chi = \begin{cases} \frac{Z}{Z_{st}} \frac{(T_{\max} - T_0)}{T_{\max}} + \frac{T_0}{T_{\max}}, & \text{if } 0 \le Z < Z_{st} \\ \frac{1 - Z}{1 - Z_{st}} \frac{(T_{\max} - T_f)}{T_{\max}} + \frac{T_f}{T_{\max}}, & \text{if } Z_{st} \le Z \le 1 \end{cases}$$
(2.41)

Generally, $T_0 \ll T_{max}$ and $T_f \ll T_{max}$. Eq. (2.41) would become

$$\chi \approx \begin{cases} \frac{Z}{Z_{st}}, & \text{if } 0 \le Z < Z_{st} \\ \frac{1-Z}{1-Z_{st}}, & \text{if } Z_{st} \le Z \le 1 \end{cases}$$

$$(2.42)$$

The mixture fraction is defined as [3]

$$Z = \frac{sY_{f_{2}} - Y_{O_{2}} + Y_{O_{2}}^{"}}{sY_{\mu}^{"} + Y_{O_{2}}^{"}}$$
(2.43)

where Y_{fu}^0 is the fuel mass fraction in the fuel stream, and $Y_{o_2}^0$ is the oxygen mass fraction in the oxidizer stream. The stoichiometric mixture fraction can be expressed as

$$Z_{\mu} = \frac{Y_{O_{2}}^{\circ}}{sY_{\mu}^{\circ} + Y_{O_{2}}^{\circ}}$$
(2.44)

Substituting Eq. (2.43) and Eq. (2.44), Eq. (2.42) would be recast as

$$\chi \approx \begin{cases} \frac{s\left(Y_{f_{u}} - \frac{Y_{O_{1}}}{s}\right) + Y_{O_{2}}^{0}}{Y_{O_{2}}^{0}}, & \text{if } Y_{f_{u}} < \frac{Y_{O_{2}}}{s} \\ \frac{Y_{f_{u}}^{0} - \left(Y_{f_{u}} - \frac{Y_{O_{1}}}{s}\right)}{Y_{f_{u}}^{0}}, & \text{if } Y_{f_{u}} \ge \frac{Y_{O_{2}}}{s} \end{cases}$$
(2.45)

Defining the reference species mass fraction $Y_{ref} = Y_{fu} - \frac{Y_{O_1}}{s}$, Eq. (2.45) would become

$$\chi \approx \begin{cases} \frac{sY_{ref} + Y_{O_{2}}^{0}}{Y_{O_{2}}^{0}}, & \text{if } Y_{ref} < 0\\ \frac{Y_{f_{n}}^{0} - Y_{ref}}{Y_{f_{n}}^{0}}, & \text{if } Y_{ref} \ge 0 \end{cases}$$
(2.46)

Hence, in LES Eq. (2.46) would be written as

$$\chi \approx \begin{cases} \frac{s\tilde{Y}_{ref} + Y_{O_{2}}^{0}}{Y_{O_{2}}^{0}}, & \text{if } \tilde{Y}_{ref} < 0\\ \frac{Y_{fu}^{0} - \tilde{Y}_{ref}}{Y_{fu}^{0}}, & \text{if } \tilde{Y}_{ref} \ge 0 \end{cases}$$
(2.47)

where $\tilde{Y}_{ref} = \tilde{Y}_{fu} - \frac{\tilde{Y}_{O_2}}{s}$.

Chapter 3

Soot Model

3.1 INTRODUCTION

It is reported that the main cause of death in fires is smoke inhalation, as an estimated 50~80% of fire deaths are associated with the presence of soot. Moreover, soot particles have considerable effect on radiative heat transfer, and further influence fire spread and fire growth. A reliable soot model is, hence, crucial to investigate fire behaviors. However, soot chemistry is a complex process involving soot inception, soot coagulation, soot agglomeration, soot surface growth, and soot oxidation. It is extremely challenging to consider all these sub-processes in numerical simulations. Moreover, a robust chemical mechanism for soot formation is still lacking for diffusion flames. There exist at least two distinct mechanisms [32, 33], i.e. C_2H_2 addition and Polycyclic Aromatic Hydrocarbon (PAH) addition. Note that the C_2H_2 addition mechanism is controlled by heterogeneous surface growth reactions, while the PAH addition mechanism is determined by homogeneous gas phase reactions. Therefore, there is still a gap between soot model and practical applications.

Ideally, a soot model needs to account for the underlying physics of nucleation/inception, surface growth, coagulation/agglomeration and oxidation. Detailed soot chemistry models [33-46] take into account multiple soot reaction equations starting from nuclei precursors to soot particles, requiring the relevant

species concentrations such as C_2H_2 and OH which can only be predicted with detailed chemistry in the combustion model. These models cannot be easily extended to relatively large scale fires due to their complexity and computational cost. On the contrary, the soot conversion factor [47-49], applied in FDS program, and state relationship method [50] are too simple to represent the soot behaviour, as the generation of soot is assumed to be proportional to the amount of fuel consumed and the dependence of temperature on the soot generation is neglected.

Semi-empirical soot models [6, 51-73] are widely used in the combustion community. These models neglect the detailed paths of soot generation. The soot nucleation, surface growth, agglomeration, coagulation, and oxidation rates are written in the Arrhenius-style. Typically, two conservation equations are solved for the soot mass fraction and soot number density. However, these models all include several fuel-specific parameters which are not easily obtainable for various fuels, and they are also significantly dependent on the specific scenario. The potential of a smoke point based model to alleviate these limitations were recognized by Markstein and De Ris [74-76] in the 1980s. The concept was further elaborated by Delichatsios [77, 78] but an applicable strategy to incorporate it in fire modelling has yet been developed.

It was almost a decade later, Lautenberger et al. [32, 79] proposed a laminar smoke-point-based soot model by explicitly neglecting the processes of nucleation, inception, coagulation and agglomeration. The soot formation and oxidation rates are assumed to be analytic functions of mixture fraction and temperature. Most importantly, the model could be generalized to the multiple hydrocarbon fuels by relating the soot formation rate to its laminar smoke point

height (SPH). Contrary to the relatively popular two-equation soot model mentioned above, the soot number density equation is eliminated here by assuming the soot formation and oxidation is independent of surface area in non-premixed hydrocarbon flames, and the model coefficients are expected to be feasible for general fuels. On the basis of this model, Beji et al. [80-82] made further improvement with the combination of earlier work of Delichatsios [78], particularly for the soot formation and its critical conditions. Both groups are now investigating effective means to extend their models to turbulent flames and fires.

As a matter of fact, these two models were originally developed for laminar flames, and the extension from laminar flames to turbulent flames is still on-going. Conditional momentum closure (CMC) is adopted in [83, 84] to treat the soot source term in turbulent flames, however, it would be very timeconsuming and thus unlikely to be applicable to fire simulations. Chatterjee [85] introduced a laminar flamelet concept potentially promising for fire simulations, but optically thin assumption during the construction of the lookup table limits its wide use at present. It is also worth pointing out that at this stage the radiative fraction of heat release rate is the only output quantity from this model. It would be difficult to conduct the complete validation study without soot volume fraction predicted, as radiative fraction is believed to be less sensitive in comparison to soot volume fraction.

The aim of this chapter is to investigate the treatment of laminar-based SPSM in the LES framework. Meanwhile, the effect of soot on the fuel distribution and energy transport will be also considered, as well as the soot yield calculation.

3.2 SMOKE POINT CONCEPT

Experimentally established flame similarity analysis [74, 78] suggests that the sooting propensity of each fuel is inversely proportional to its laminar SPH. With the help of this SPH, the soot model developed from one fuel type could be extended to the general fuel.

Theoretically, SPH is defined as the height of a laminar diffusion flame at which the flame breaks open at its apex and emits a stream of smoke [86]. The SPH of some typical fuels are listed in Table 3.1, and more SPH data of hydrocarbon fuels could be found in Refs. [79, 81, 83, 86-89].

Luel type	Smoke point height (m)
Methanol	œ
Methane	0.29
Ethane	0.243
Propane	0.162
Heptane	0.125
Ethylene	0.106
Propylene	0.029
Toluene	0.008

Table 3.1 Smoke point height data

It should be noted that methane is generally thought to not have a smoke point since the flame becomes turbulent before it emits smoke. Methane may even play a role in suppressing soot formation if it is included in fuel mixtures as indicated in Ref. [76]. However, Lautenberger [79] assigned a smoke point height of 29cm, and subsequently Beji [81] and Yao [83] followed this assignment in their soot model developments. This value is believed to be estimated from the comparison of radiative fraction between the methane and ethane flame. In this study, the same value is applied.

3.3 LAMINAR SMOKE POINT MODEL

In laminar soot modelling, a transport equation for soot mass fraction (Y_{r}) is written as

$$\frac{\partial \rho Y_{s}}{\partial t} + \frac{\partial \rho u_{j} Y_{s}}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left(0.556 Y_{s} \frac{\mu}{T} \frac{\partial T}{\partial x_{j}} \right) + \frac{\partial}{\partial x_{j}} \left(\rho D_{s} \frac{\partial Y_{s}}{\partial x_{j}} \right) + \omega_{s,f} + \omega_{s,o}$$
(3.1)

The first term on the RHS of Eq. (3.1) represents the thermophoretic effect, causing soot diffusion along temperature gradient. It is recommended in [56] that the soot diffusivity (D_r) is taken as 1% of gas diffusivity in order to reduce the numerical fluctuations. In fact, the key issue would be the expression of soot generation rate (ω_r). The laminar soot model in Ref. [82], which is based on the smoke point concept, is introduced as the base soot model in this study:

$$\omega_{s,f} = \begin{cases} \frac{A_f}{L_{sp}} \rho^2 \left(Y_{fs}^0 \frac{Z - Z_{st}}{1 - Z_{st}} \right) T' \exp\left(-\frac{T_a}{T}\right), & Z_{s,o} \le Z \le Z_{s,f} \\ 0, & else \end{cases}$$
(3.2)

$$\omega_{s,o} = \begin{cases} -\frac{A_o}{L_{sp}}, & Z \le Z_{s,o} \text{ and } T \ge 1300K\\ 0, & else \end{cases}$$
(3.3)

where A_f and A_o are fuel-independent constants for soot formation and oxidation, chosen as 4.4E-6 and 0.11 [82], respectively. r is fuel-independent exponential factor for temperature, set as 2.25 [82]. T_a is fuel-independent activation temperature for soot formation, selected as 2000 K [82]. Y_{fa}^0 is fuel mass fraction in fuel stream. $Z_{s,f}$ and $Z_{s,o}$ are critical mixture fractions for soot formation and oxidation, respectively, and they could be normalized by the stoichiometric mixture fraction $(Z_{s,f})$ [32, 82]:

$$Z_{s,f} = \psi_{s,f} Z_{st} \tag{3.4}$$

$$Z_{s,o} = \psi_{s,o} Z_{st} \tag{3.5}$$

where $\Psi_{s,f}$ and $\Psi_{s,o}$ are assumed as fuel-independent constants, chosen as 2.5 [82] and 1, respectively.

Note that a constant volumetric oxidation rate is developed in the base study [82], so the independence of soot oxidation on the surface area is implied based on detailed experiments of soot production in laminar non-premixed flames [32, 78, 82].

3.3.1 Conversion of Mixture Fraction

Mixture fraction transport equation is not solved in this study, and fuel mass fraction and oxygen mass fraction are determined directly from their transport equations. It would be necessary to eliminate the mixture fraction in the above soot model by using the definition of mixture fraction, i.e. Eq. (2.43):

$$\omega_{s.f} = \begin{cases} \frac{A_f}{L_{sp}} \rho^2 Y_{fu} T' \exp\left(-\frac{T_a}{T}\right), & \frac{(\psi_{s.o} - 1)Y_{O_1}^{\circ}}{s} \le Y_{fu} - \frac{Y_{O_1}}{s} \le \frac{(\psi_{s.f} - 1)Y_{O_1}^{\circ}}{s} \\ 0, & else \end{cases}$$
(3.6)

$$\omega_{s,o} = \begin{cases} -\frac{A_o}{L_{sp}}, & Y_{fu} - \frac{Y_{O_1}}{s} \le \frac{(\psi_{s,o} - 1)Y_{O_1}^{\circ}}{s} \text{ and } T \ge 1300K \\ 0, & else \end{cases}$$
(3.7)

In some CFD code such as FDS, mixture fraction is used to derive the fuel and oxygen mass fraction according to the assumption of Burke-Schumann flame structure [3], i.e. "mixed is burnt", in order to decrease the number of variables. However, the mixture fraction would not be conserved if the effect of soot formation on the fuel mass fraction is introduced, and the conversion of mixture fraction would be helpful to resolve this issue, as discussed later.

3.4 TURBULENT SMOKE POINT MODEL

It is well acknowledged that turbulence would influence the flame structure, as well as the soot formation and oxidation processes. In turbulent flames, the fluctuation of soot volume fraction may be considerable and even comparable to the time-averaged property. Generally, the instantancous soot mass fraction transport equation (i.e. Eq. (3.1)), which is suitable for laminar flame simulations, could not be applied to turbulent flames directly. The following sections would describe the procedures to account for the effect of turbulence on soot generation, which a new model is developed for.

3.4.1 Favre Averaging

In LES, a spatial filtering process would be applied to Eq. (3.1) to mimic the sub-grid scale influence on the grid scale properties:

$$\frac{\partial \overline{\rho} \widetilde{Y}_{,i}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_{,i} \widetilde{Y}_{,i}}{\partial x_{,i}} = \frac{\partial}{\partial x_{,i}} \left[\overline{\rho} \left(\widetilde{u}_{,i} \widetilde{Y}_{,i} - \widetilde{u}_{,i} \widetilde{Y}_{,i} \right) \right] + \frac{\partial}{\partial x_{,i}} \left(0.556 Y_{,i} \frac{\mu}{T} \frac{\partial T}{\partial x_{,i}} \right) + \frac{\partial}{\partial x_{,i}} \left(\overline{\rho} D_{,i} \frac{\partial Y_{,i}}{\partial x_{,i}} \right) + \overline{\omega}_{,i,i} + \overline{\omega}_{,i,i} (3.8)$$

$$\overline{\phi(\mathbf{x},t)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(\mathbf{x}',t) F(\mathbf{x},\mathbf{x}',\Delta) dx_1' dx_2' dx_3'$$
(3.9)

$$\overline{\rho}\widetilde{\phi(\mathbf{x},t)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho\phi(\mathbf{x}',t) F(\mathbf{x},\mathbf{x}',\Delta) dx_1' dx_2' dx_3'$$
(3.10)

where F is a filtering function for LES, independent of position x; bar and tilde mean spacial filtering and mass-weighted Favre filtering, respectively. In fact, the filtering process is not preformed explicitly with a filtering function, and it is adopted here in order to achieve the soot mass fraction transport equation for LES.

Unresolved scalar flux (first term of RHS) are often described as

$$\widetilde{u_{i}}\widetilde{Y_{s}} - \widetilde{u_{i}}\widetilde{Y_{s}} = \frac{\upsilon_{i}}{Sc_{i}}\frac{\partial\widetilde{Y_{s}}}{\partial x_{i}}$$
(3.11)

where v_i is turbulent viscosity obtained from SGS turbulence model; Sc_i is turbulent Schmidt number. Thermophoretic effect (second term of RHS), reflecting the soot molecular diffusion due to temperature gradient, is believed to be relatively small in comparison with turbulent mixing. Moreover, the thermophoretic term is determined to be non-linear, and it is hard to model this term in LES. An alternative way to estimate the effect of this term would be DNS, which is beyond the scope of this study. Therefore, it is neglected following other relevant studies [65, 84]. The filtered laminar diffusion flux (third term of RHS) may be modelled through a simple gradient assumption, such as

$$\overline{\rho D_{r} \frac{\partial Y_{s}}{\partial x_{j}}} = \overline{\rho} D_{r} \frac{\partial \widetilde{Y}_{s}}{\partial x_{j}}$$
(3.12)

The key issue here would be the treatment of soot source term in LES, which is the main driver for soot generation. It is true that the accuracy of the predicted soot volume fraction is mainly attributed to this term, particularly in the near-field of a fire. The method to tackle this issue is described in detail in the following sections.

3.4.2 Soot Formation

3.4.2.1 Partially Stirred Reactor

The concept of partially stirred reactor (PaSR) [43, 90, 91] is applied for the soot formation term to account for the turbulence/chemistry interaction. A computational cell is split into two different zones as shown in Fig. 3.1. The shaded area reflects the reacting zone, while the other area means the nonreacting zone. Note that the shape of the reacting zone in Fig. 3.1 is schematic, so it doesn't depict the real structure of this zone. In this study, soot formation process, which is relatively slow, is assumed to take place only in this reacting zone. In this zone, the composition is supposed to be homogenous, allowing us to disregard any fluctuations when calculating the soot formation rate. The typical length scale of this zone is still unclear in the turbulent energy cascade. In contrast, soot formation will not proceed in the non-reacting zone, and the turbulent mixing effect is thus dominant there.



Fig. 3.1 Schematic of PaSR concept

In Fig. 3.1, $\widetilde{Y_s^0}$ means the mass weighted soot mass fraction at previous time step, while $\widetilde{Y_s^1}$ denotes the mass fraction at current time step. It is noted that $\widetilde{Y_s^0}$ and $\widetilde{Y_s^1}$ are the integrated variables over a whole cell. In contrast, Y_s^1 is the

local soot mass fraction in the reacting zone. The whole process, from \widetilde{Y}_{s}^{0} at the previous time step to \widetilde{Y}_{s} at the current time step, could be divided into two substeps [90] proceeding in parallel, as described in Fig. 3.2. It could be summarized as follows:

- Sub-Step I: the previous $\widetilde{Y_s^0}$ changes to r; due to the soot formation in the reacting zone;
- > Sub-step II: the newly formed Y_s mixes with non-reacting part \widetilde{Y}_s^0 through turbulence, resulting in \widetilde{Y}_s^1 .



Fig. 3.2 Schematic of \tilde{Y}_{s}^{i} evolvement in PaSR

Like the treatment in [90], the filtered soot formation rate may be expressed as

$$\overline{\omega}_{i,f} = \overline{\rho} \, \frac{\widetilde{Y}_i^* - \widetilde{Y}_i^1}{r_{mit}} = \omega_{i,f}^* \tag{3.13}$$

where r_{mn} is turbulent mixing time scale. $\omega_{s,f}$ indicates the intermediate soot formation rate obtained from the properties in the reacting zone. It is illustrated that the expression of Eq. (3.13) is analogous to the one in the EDC combustion model. As the irreversible fast chemistry is assumed in EDC, the mass fraction would be zero for some species, which is dependent on the reacting mixture. For instance, the fuel mass fraction will be zero for the lean mixture. Hence, the filtered reaction rate could be directly achieved for the species source term, like the treatment in the previous section. However, \widetilde{Y}_{r}^{*} is unlikely to be achieved due to the relatively slow chemistry of soot generation, if the detailed paths are not included. Thus, the filtered soot formation rate is not straightforward.

According to [43, 90, 91], $\omega_{s,f}$ may be transformed as

$$\boldsymbol{\omega}_{s,f}^{*} = \boldsymbol{\kappa} \boldsymbol{\omega}_{s,f}^{1} \tag{3.14}$$

$$\kappa = \frac{\tau_{c,r}}{\tau_{c,r} + \tau_{min}} \tag{3.15}$$

Here $\omega_{s,f}^{1}$ is linked to the soot formation rate, i.e. $\omega_{s,f}^{1}$, calculated from the filtered properties at current time step. κ can be regarded as the mass fraction occupied by the reacting zone in a cell. $\tau_{c,r}$ and τ_{min} are chemical time scale and turbulent mixture time scale, respectively, which will be discussed in the following subsections. In this study, $\omega_{s,f}^{1}$ is assumed to be

$$\omega_{s,f}^{\dagger} = \omega_{s,f} \left(\tilde{Y}_{\mu}, \tilde{Y}_{\nu}, \tilde{T} \right)$$
(3.16)

Note that the implicit scheme needs to be included to mimic the relevant properties at the current time step.

Combining Eqs. (3.6), (3.13), (3.14) and (3.16), the filtered soot formation rate would be

$$\overline{\omega}_{s,f} = \begin{cases} \kappa \frac{A_f}{L_{sp}} \overline{\rho}^2 \widetilde{Y}_{fu} \widetilde{T}' \exp\left(-\frac{T_a}{\widetilde{T}}\right), & \frac{(\psi_{s,a}-1)Y_{o_1}^{\circ}}{s} \le \widetilde{Y}_{fu} - \frac{\widetilde{Y}_{o_1}}{s} \le \frac{(\psi_{s,f}-1)Y_{o_1}^{\circ}}{s} \\ 0, & else \end{cases}$$
(3.17)

3.4.2.2 Time Scales

Instead of calculating the soot chemical time scale with the detailed chemistry [43, 90, 91], this variable is assumed to be proportional to the laminar SPH of the fuel [78, 82, 84]:

$$\tau_{c,s} = C_{sp} L_{sp} \tag{3.18}$$

The characteristic soot production time scale of ethylene diffusion flame is chosen to be 40 ms according to the detailed peak soot volume fraction distributions as a function of the residence time [92]. Given the laminar SPH of ethylene is 0.11 m [82], C_{ip} is calculated to be 0.364 based on Eq. (3.18). Note that the effect of turbulence on this chemical time scale is not considered here.

The turbulent mixing time scale for soot formation is supposed to be the geometric mean of Kolmogorov time scale (τ_{η}) and integral time scale (τ_{l}), written as

$$\tau_{mix} = \sqrt{\tau_{\eta}\tau_{l}} \tag{3.19}$$

3.4.2.3 Roadmap

As the detailed roadmap of soot particles originating from precursors is unknown here, it is impossible to include exactly the heats of formation in the energy transport equation. Luckily, the magnitude of this term seem to be small by comparing with the fuel-generated heat, so it is less likely that this term influences hugely the major parameters such as mean temperature and velocity distributions. However, the soot-induced fuel loss should be considered in the simulations, particularly for high-sooty flames, as this fuel loss would result in the deviation of global single-step kinetics. In this study, the chemical equation of soot formation is assumed as

$$C_{x}H_{y}(g) \rightarrow C_{x}H_{y}(s) - \Delta h_{f,s}$$
(3.20)

Note that the composition of soot particles is supposed to be the same as the fuel, like the relative treatment in [32]. $\Delta h_{f,s}$ is the heat released in phase transformation from gas-phase fuel to solid-phase particles, theoretically including the specific latent heat of fusion and heat of vaporization. According to the mass balance of Eq. (3.20), the filtered fuel loss rate due to soot formation $(\bar{\omega}_{h,s})$ would be

$$\bar{\omega}_{j_{k},j} = -\bar{\omega}_{j,j} \tag{3.21}$$

The consumption or production rate of other species (O_2 , CO_2 , and H_2O) would not be influenced by soot generation:

$$\bar{a}_{0,s} = 0; \ \bar{a}_{0,s} = 0; \ \bar{a}_{H_{2}0,s} = 0$$
 (3.22)

Note that it is hard to obtain the released energy in Eq. (3.20), as solidphase and liquid-phase thermo-physical properties are normally not included in fire simulations. Therefore, this energy is not added to the total gas enthalpy in the energy transport equation. Furthermore, the combustion would be incomplete, as part of the fuel is supposed to be converted into soot particles directly. Thus, the heat released is associated with only a portion of the fuel consumption as discussed below.

3.4.3 Soot Oxidation

With the concept of PaSR, the filtered soot oxidation rate in turbulent flames might be expressed as follows based on the constant volumetric oxidation rate in the original work [82]:

$$\overline{\omega}_{s,o} = \begin{cases} -\kappa \frac{A_o}{L_{sp}}, \quad Y_{fu} - \frac{Y_{O_s}}{s} \le \frac{(\psi_{s,o} - 1)Y_{O_s}^\circ}{s} \text{ and } T \ge 1300K \\ 0, \quad else \end{cases}$$
(3.23)

This expression is tested during pool fire simulations, and unfortunately numerical instability is observed in the soot oxidation region. The reason is associated with the over-prediction of soot oxidation at some locations, giving rise to the negative value of soot mass fraction. A laminar soot oxidation model [32] coupled with PaSR is also examined in turbulent non-premixed flames, and numerical instability is also encountered. These two original oxidation models have something in common: the profile of oxidation rate varying with the mixture fraction in the soot oxidation region is pre-determined rather than computed during simulations. This pre-assumed profile would be inappropriate in some oxidation region, resulting in unreasonable predictions of soot mass fraction. Therefore, a new soot oxidation model is developed here.

According to Eq. (3.20), the chemical equation for soot oxidation is assumed as

$$C_{x}H_{y}(s) + \left(x + \frac{y}{4}\right)O_{2} \rightarrow xCO_{2} + \frac{y}{2}H_{2}O - \Delta h_{c,s}$$

$$(3.24)$$

which is quite similar to the fuel reaction equation in the combustion model. It might be possible to apply the EDC based fuel reaction rate to soot oxidation. Furthermore, oxygen is highly likely to be sufficient in the soot oxidation region $(\tilde{Y}_{j_{w}} - \frac{\tilde{Y}_{o_{1}}}{s} \le \frac{(\psi_{s,v} - 1)Y_{o_{1}}^{*}}{s}$ and $\tilde{T} \ge 1300K$), and soot would thus be a dominant species to limit the oxidation rate. Therefore, soot oxidation rate may be expressed as

$$\vec{\omega}_{s,o} = \begin{cases} -\vec{\rho}\vec{Y}_{s}\vec{m}\cdot\frac{\gamma\chi}{1-\gamma\chi}, \quad \vec{Y}_{fu} - \frac{\vec{Y}_{O_{s}}}{s} \le \frac{(\psi_{s,o}-1)Y_{O_{s}}^{\circ}}{s} \text{ and } \vec{T} \ge 1300K \\ 0, \quad else \end{cases}$$
(3.25)

Note that Eq. (3.25) is associated with soot mass fraction. If soot mass fraction is small, the relevant oxidation rate will be small correspondingly, avoiding the risk of numerical instability.

Moreover, Eq. (3.25) implies that soot oxidation is assumed to proceed infinitely fast, distinct from the soot formation process where a partially stirred reactor is involved. One may further assume that the turbulent mixing time scale for the soot oxidation process is equivalent to the one for soot formation, and then Eq. (3.25) may be written as

$$\overline{\omega}_{s,o} = \begin{cases} -\frac{\overline{\rho}\widetilde{Y}_{s}}{\tau_{mix}} \frac{\gamma\chi}{1-\gamma\chi}, & \widetilde{Y}_{fu} - \frac{\widetilde{Y}_{O_{s}}}{s} \le \frac{(\psi_{s,o}-1)Y_{O_{s}}^{\circ}}{s} \text{ and } \widetilde{T} \ge 1300K\\ 0, & else \end{cases}$$
(3.26)

In this study, both Eq. (3.25) and Eq. (3.26) are included, and their effects on the soot volume fraction distributions are investigated in Chapter 6.

3.4.3.1 Roadmap

Based on mass balance of Eq. (3.24), the consumption or production rate of relevant species (O_2 , CO_2 , and H_2O) would be calculated from

$$\overline{\omega}_{o_1.so} = \left(x + \frac{y}{4}\right) \frac{MW_{o_1}}{MW_{in}} \overline{\omega}_{s,o}$$
(3.27)

$$\overline{\omega}_{CO_{1,10}} = -x \frac{MW_{CO_{1}}}{MW_{I_{4}}} \overline{\omega}_{s,0}$$
(3.28)

$$\overline{\omega}_{H_1O,so} = -\frac{y}{2} \frac{MW_{H_1O}}{MW_{fu}} \overline{\omega}_{s,o}$$
(3.29)

Furthermore, the soot oxidation process would not affect the fuel distribution directly. Thus,

$$\bar{\omega}_{fu,so} = 0 \tag{3.30}$$

Given energy balance, the heat released from Eq. (3.24) would be

$$\Delta h_{c,s} = \Delta h_c - \Delta h_{f,s} \tag{3.31}$$

Similar to the treatment in the above section, $\Delta h_{f,s}$ is also neglected here. Thus,

$$\Delta h_{cs} \approx \Delta h_c \tag{3.32}$$

Generally, soot particles are assumed to be "extra fuel packs" in most circumstances, where those particles have same characteristics as fuel, like temperature and velocity. In contrast, they are considered as condensed particles during the calculation of soot volume fraction. Soot diffusion is normally much weaker than the one for gas species.

3.4.4 Soot Energy Treatment

It is assumed that some energy is still stored in soot particles due to the incomplete combustion, while all energy would have been released if the combustion is complete. The energy potentially hidden in soot particles would be

$$Q_{s,form} = \int_{V} \overline{\omega}_{s,f} \Delta h_{c,s} dV$$
(3.33)

Some part of soot particles is oxidized when oxygen is rich, releasing a portion of the hidden energy:

$$Q_{s,\text{oxid}} = -\int \bar{\omega}_{s,o} \Delta h_{c,s} dV \tag{3.34}$$

Therefore, the net potential energy hidden in soot particles would be,

$$Q_s = Q_{s,orm} - Q_{s,oxid} \tag{3.35}$$

The predicted heat release rate (Q) is composed of two parts: 1) heat released from gas phase fuel combustion with the reaction rate obtained from the EDC combustion model; 2) heat released from the oxidation of "solid" phase soot particles. Thus,

$$Q = Q_{s,axid} + \int_{v} \overline{\omega}_{fu,g} \Delta h_c dV$$
(3.36)

The total energy based on the consumption of fuel would then be

$$Q_t = Q + Q_s \tag{3.37}$$

This variable could also be described as

$$Q = \dot{m}_{h}\Delta h_c \tag{3.38}$$

where \dot{m}_{fu} is the inlet fuel flow rate. During calculations, Eq. (3.37) and Eq. (3.38) are monitored in order to evaluate the convergence of total energy.

3.4.5 Soot Yield

Soot yield (λ_r) is defined as the fraction of the fuel converted to soot particles. Note that Tewarson [86] expressed this quantity as a function of the laminar smoke point height, suggesting that it is only dependent on the fuel type. According to the above definition it may be calculated as

$$\lambda_{s} = \frac{\int (\bar{\omega}_{s,f} + \bar{\omega}_{s,o}) dV}{\int (\bar{\omega}_{s,f} + \bar{\omega}_{fu,g}) dV}$$
(3.39)

It is found that the value of soot yield estimated from Eq. (3.39) might be negative if soot oxidation is too intensive during some iterations. However, the time-averaged soot yield is always positive, reflecting the conversion of fuel to soot.

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Chapter 4

Radiation Model

4.1 INTRODUCTION

It has long been recognized [93] that radiation is a dominant mode of heat transfer in fires of very large scale, affecting the fire growth and spread. Thus, the corresponding radiation model should be considered very carefully. At present, four radiation models, including "P1", "DTM", "DOM" and "FVM", are mainly used in the combustion community. "P1" is the simplest case of the more general P-N method [94-96], based on the expansion of the radiation intensity into an orthogonal series of spherical harmonics. This model can deliver the reasonable estimation of radiation loss term in energy transport equation, only if the optical thickness is very large. "DTM" implies discrete transfer method [94-98], and it divides energy emitted into the hemisphere into finite number of rays and assumes that the radiation leaving the surface element in a certain range of solid angles can be approximated by the single ray. Note that this model is principally built on the concept of solving representative rays in a radiating enclosure, and the directions of the rays has to be pre-specified in advance rather than being chosen at random. "DOM" means discrete ordinate method [94-96, 99, 100], and it solves radiative transport equations (RTE) over a finite number of discrete directions. Note that quadratures sets, including ordinate directions and angular weights, need to be generated accurately, and the products of the angular

directions and their weights should satisfy certain full-range and half-range moment constraints [94, 95, 99]. "FVM", which represents finite volume method [94-96, 99, 101-103], could avoid that issue, and it is believed to be sophisticated enough for the fire simulations [48]. Additionally, Monte Carlo method [94-96] is rarely utilized in the fire community, due to its complexity and the corresponding computational cost.

In this study, the finite volume method will be introduced to discretize the radiative transfer equations (RTE) in the non-optically thin flames, while the optically thin assumption will be made for optically thin flames to avoid the solution of the spectral RTE. Moreover, three different methods will be developed to calculate the surface emissive power (SEP), which is extremely important in the large scale LNG fires.

4.2 RADIATIVE TRANSPORT EQUATIONS

The radiative transport equations for an absorbing/emitting and scattering medium could be expressed as [94]

$$\hat{s} \cdot \nabla I_{n}(x,\hat{s}) = \kappa_{n}(x) I_{b,n}(x) - \beta_{n}(x) I_{n}(x,\hat{s}) + \frac{\sigma_{n}(x)}{4\pi} \int_{4\pi} I_{n}(x,\hat{s}') \Phi_{n}(x,\hat{s},\hat{s}') d\Omega' \quad (4.1)$$

$$\beta_n(\mathbf{x}) = \kappa_n(\mathbf{x}) + \sigma_n(\mathbf{x}) \tag{4.2}$$

where the bold x stands for the spacial locations, \hat{s} is the direction vector of the intensity, $I_n(x,\hat{s})$ is the radiation intensity integrated over the spectral band n covering a portion of wavelength, $\beta_n(x)$ is the local spectral extinction coefficient, $\kappa_n(x)$ is the local spectral absorption coefficient, $\sigma_n(x)$ is the local spectral scattering coefficient, $\Phi_n(x,\hat{s},\hat{s}')$ is the local spectral scattering phase function, $d\Omega$ is the solid angle. The source term $I_{b,n}(x)$ could be written as a fraction of blackbody radiation [48, 94]:

$$I_{b,n} = F_n(\lambda_{n,\min}, \lambda_{n,\max})\sigma \tilde{T}^4(\mathbf{x})/\pi$$
(4.3)

where σ is the Stefan-Boltzmann constant, 5.67×10^{-8} W/m²K⁴. The calculation of F_n over the band *n* with the wavelength ranging from $\lambda_{n,\min}$ to $\lambda_{n,\max}$ is detailed in Ref. [94].

The total intensity $(I(x,\hat{s}))$ is calculated by summing the intensities over all the bands:

$$I(\mathbf{x},\hat{s}) = \sum_{n} I_n(\mathbf{x},\hat{s})$$
(4.4)

The incident radiation (G(x)) is defined as

$$G(\mathbf{x}) = \int_{4\pi} I(\mathbf{x}, \hat{s}) d\Omega$$
 (4.5)

The net radiant heat flux vector $(q_r''(x))$ would be

$$q_r''(\mathbf{x}) = \int_{4\pi} \hat{s} l(\mathbf{x}, \hat{s}) d\Omega$$
(4.6)

The incident heat flux $(q_{in}^{*}(x))$ to a surface with the normal vector \hat{n} would be

$$q_{in}^{n}(\mathbf{x}) = \int_{\hat{s}\cdot\hat{n}<0} I(\mathbf{x},\hat{s}) |\hat{s}\cdot\hat{n}| d\Omega \qquad (4.7)$$

In contrast, the out-going heat flux $(q_{out}^{*}(x))$ from that surface would be

$$q_{out}^{*}(\mathbf{x}) = \int_{\hat{s}, \hat{n} > 0} I(\mathbf{x}, \hat{s})(\hat{s} \cdot \hat{n}) d\Omega \qquad (4.8)$$

4.2.1 Absorption Coefficient

The local spectral absorption coefficient (κ_n) depends on the composition of species, the temperature and the spectral band. In a fire, the combustion products consist of gas species and soot particles, and thus κ_n could be decomposed into the gas absorption coefficient $(\kappa_{n,s})$ and the soot absorption coefficient $(\kappa_{n,s})$:

$$\kappa_n = \kappa_{n,g} + \kappa_{n,s} \tag{4.9}$$

The $\kappa_{n,s}$ would change rapidly due to its dependence on the spectral band, giving rise to the main difficulty for the calculation. Here the RADCAL program [104] is introduced for this coefficient. In this program, the spectral bands are predefined according to the critical wavelengths, and the species involved with the absorption would thus be known for each band. Based on the concentrations of the corresponding species as well as the temperature, the spectral absorption coefficient over each band would be determined as follows:

$$\kappa_{n,g} = \sum_{m} a_{p,m} p_m \tag{4.10}$$

where *m* indicates the species over the band *n*. $a_{p,m}$ is the Planck-mean absorption coefficient for the species *m*, and it could be expressed as polynomials in temperature according to the RADCAL program, as shown in Fig. 4.1. One can also find the detailed mathematical expressions in Ref. [105]. p_m is the partial pressure of the species *m*, written as

$$p_m = \overline{p} \tilde{Y}_m \tag{4.11}$$



Fig. 4.1 Planck-mean gas absorption coefficient against temperature

Unlike the gas species, the radiation spectrum of soot is continuous, and $\kappa_{n,r}$ may thus be assumed to be the same over all the bands considered. Felske and Tien [94, 106] suggested using an average value of Planck-mean and Rosseland-mean absorption coefficients for $\kappa_{n,r}$ in all optical regimes:

$$\kappa_{ns} = 3.72 f_{\nu} C_0 \tilde{T} / C_2 \tag{4.12}$$

where C_2 is the second Planck function constant, 0.014388 mK. f_i is the soot volume fraction, obtained from

$$f_{v} = \frac{\overline{\rho}\overline{Y}_{i}}{\rho_{i}}$$
(4.13)

where ρ_s is the soot density, 1800kg/m³. C_0 is a constant relying only on the soot index of refraction (a - ib):

$$C_0 = \frac{36\pi ab}{\left(a^2 - b^2 + 2\right)^2 + 4a^2b^2}$$
(4.14)

The variation of refractive index (a) and absorptive index (b) as a function of wavelength for different compositions of soot particles is elaborated in Ref. [94].

By choosing appropriate spectral average values for a and b based on the corresponding measurements, one may approximate the pre-described coefficient C_0 for Eq. (4.12).

In the fire community, the following formulation developed in Ref. [32] is widely used for $\kappa_{n,i}$:

$$\kappa_{ns} = 1226 f_v \tilde{T} \tag{4.15}$$

According to Eq. (4.12), C_0 is implicitly set as 4.74 within Eq. (4.15). In this study, Eq. (4.15) is also employed.

4.2.2 Scattering Coefficient

The scattering of thermal radiation due to soot particles is dependent on the wavelength. To solve the radiative transport equation, theoretically σ_n should be calculated for each spectral band. In fact, this coefficient is generally very small compared to the absorption coefficient [94], and σ_n is thus neglected in this work, similar to the treatment in other studies [32, 82, 84, 85]. Hence, Eq. (4.1) would be simplified as

$$\hat{s} \cdot \nabla I_n(\mathbf{x}, \hat{s}) = \kappa_n(\mathbf{x}) I_{b,n}(\mathbf{x}) - \kappa_n(\mathbf{x}) I_n(\mathbf{x}, \hat{s})$$

$$(4.16)$$

Moreover, the scattering phase function $\Phi(x, \hat{s}, \hat{s}')$ in Eq. (4.1) is associated with different directions of intensity, and it would thus be very difficult to compute this term. The treatment of neglecting the scattering coefficient could also bypass this issue.

4.3 SOLUTION METHOD

In this study, there are two approaches to account for the radiation source term in the energy transport equation. One is based on the optically thin assumption, while the other one is reliant on the finite volume method. The details about these two approaches are elaborated as follows.

4.3.1 Optically Thin Assumption

For optically thin flames such as methanol and methane fires, the amount of soot is relatively small in the combustion products, in comparison with the gaseous species concentration of CO_2 and H_2O . Theoretically, the spectral radiative transfer equations, i.e. Eq. (4.16), should be resolved over all the bands, and there should be enough spectral bands to cover the most important radiative wavelengths of CO_2 and H_2O , leading to the fact that it would be very timeconsuming to achieve the radiation source term.

Sandia National Laboratories developed an alternative method [105, 107] to deal with this kind of optically thin flames, expressed as

$$-\nabla \cdot q_r''(\mathbf{x}) = -4\sigma\kappa(\mathbf{x}) \left(\tilde{T}^4(\mathbf{x}) - T_b^4(\mathbf{x}) \right)$$
(4.17)

where $T_b(x)$ is the background temperature. One can realise that $I_n(x,\hat{s})$ is not involved within Eq. (4.17), and therefore the solution of the spectral RTE is avoided here. Note that this optically thin assumption may slightly over-predict the radiation loss, as the incident radiation is implicitly neglected.

4.3.2 Finite Volume Method

In non-optically thin fires soot particles play a dominant role, relative to gas species in radiative heat transfer, and it is possible to assume that the fire mixture behaves as a gray medium, as soot would emit or absorb energy continuously. According to this assumption, the spectral properties, such as I_n , $I_{b,n}$ and κ_n , would not be dependent on the bands, but lumped into the total properties. Therefore, Eq. (4.16) would be further simplified as [48, 94]

$$\hat{s} \cdot \nabla I(\mathbf{x}, \hat{s}) = \kappa(\mathbf{x}) I_b(\mathbf{x}) - \kappa(\mathbf{x}) I(\mathbf{x}, \hat{s})$$
(4.18)

where $\kappa(x)$ would be obtained from

$$\kappa(\mathbf{x}) = 1226 f_{\mathbf{x}} \tilde{T} + \sum_{M} a_{p,M} p_{M}$$
(4.19)

Note that the subscript *M* denotes the gas species in the fire mixtures, distinct from *m* in Eq. (4.10). The radiation loss term $(-\nabla \cdot q_r^{"}(x))$ in the energy equation would be

$$-\nabla \cdot q_r'(\mathbf{x}) = \kappa(\mathbf{x}) G(\mathbf{x}) - 4\kappa(\mathbf{x}) \sigma T^4(\mathbf{x})$$
(4.20)

In this study, Eq. (4.18) is discretized and solved using the finite volume method (FVM), similar to the one for governing equations of fire dynamics. The concept of this method is that: the unit sphere representing all radiation directions is divided into a finite number of solid angles, and the radiative intensity is assumed to be same in each solid angle. In each grid cell, the discretized format of the RTE in each solid angle would be derived by integrating the RTE over the volume of this cell and over this solid angle. More details of this method can be

found in Refs. [94, 99, 102], and we don't elaborate it here as it is not the aim of this thesis.

4.4 SURFACE EMISSIVE POWER

The surface emissive power (SEP) is a variable representing the radiant heat flux on the flame surface. Typically, this variable is significant in large scale LNG pool fires, as discussed in the following section. In this study, three different methods are developed to calculate SEP: flame emissivity, surface heat flux, and surface emissivity.

4.4.1 Flame Emissivity

In this method, the surface emissive power would be determined based on the averaged flame emissivity over the entire flame, as well as the averaged flame temperature, and it can be expressed as

$$SEP_F = e_F \sigma T_F^4 \tag{4.21}$$

where e_r and T_r are the averaged emissivity and temperature over the whole flame, respectively. *SEP_r* stands for the calculated SEP using this method. First of all, the cells located inside the flame envelope needs to be identified. For nonsooty flames, the criterion to distinguish those cells would be associated with the local reference species mass fraction, i.e. $\tilde{Y}_{ref} \ge 0$. In contrast, the soot effect must be considered in the sooty flames. It is known that the soot oxidation process would proceed outside the gas phase combustion in our soot model, and soot particles would thus compete with remaining fuel to burn oxygen. Therefore, the criterion may become

$$\tilde{Y}_s + \tilde{Y}_{ref} \ge 0 \tag{4.22}$$

In Eq. (4.21), the averaged flame temperature T_F could be expressed as

$$T_{F} = \frac{\sum_{cell} \tilde{T}_{cell} dV_{cell}}{\sum_{cell} dV_{cell}} \bigg|_{\dot{Y}_{c} + \dot{Y}_{ref} \ge 0}$$
(4.23)

Note that the weight of volume is introduced here for the averaging process. The subscript *cell* refers to the local variable on a cell inside the flame envelope. Similarly, e_r could be written as

$$e_F = 1 - \exp(-\kappa_F L_b) \tag{4.24}$$

$$\kappa_{F} = \frac{\sum_{cell} \kappa_{cell} dV_{cell}}{\sum_{cell} dV_{cell}} \bigg|_{\dot{Y}_{i} + \dot{Y}_{rel} \ge 0}$$
(4.25)

where L_{i} is the beam length for the entire flame, expressed as

$$L_{b} = \begin{cases} \frac{4V_{F}}{A_{F}}, & \text{if optically thin} \\ \frac{3.6V_{F}}{A_{F}}, & \text{else} \end{cases}$$
(4.26)

 V_F and A_F are the volume and surface area of the flame, respectively. Bear in mind that it would be very difficult to calculate the flame surface area A_F . In fact, the exact flame sheet is really thin, and it is unlikely that all the parts of flame sheet would be captured during the simulations. Moreover, multiple layers of flame sheet may be taken somewhere. Hence, the loss or gain of parts of flame sheet is unavoidable, leading to the wrong prediction of flame surface area.

In this study, the flame is assumed to be a cylinder, as shown in Fig. 4.2. The height of the cylinder is equal to the flame height, while the diameter is equivalent to the pool size. The cylinder would be tilted in case of cross wind, as described in Fig. 4.2.b. Note that the procedures of calculating the flame height (L_f) and flame tilted angle from vertical direction (θ) are included in the next chapter. In fact, this cylindrical assumption is popularly made during the estimation of view factor in order to obtain the measured SEP from the radiometer readings in the LNG tests [108], as the flame sheet is wrinkly and always changing against time. According to this assumption, V_F and A_F in Eq. (4.26) would be expressed as

$$V_F = \frac{\pi D^2}{4} L_f$$
 (4.27)

$$A_F = \pi D L_f + \frac{\pi D^2}{4} \tag{4.28}$$

Actually, in the large scale fires this assumption will not have a big impact on the calculation of SEP, i.e. Eq. (4.21), as the averaged flame emissivity would be really close to 1 [109], as shown in Chapter 7.



Fig. 4.2 Schematic of cylindrical flame assumption (a. no cross wind; b. cross

wind)

4.4.2 Surface Heat Flux

This method aims to mimic the radiant heat flux on the flame surface. The local surface emissive power is assumed to be same as the out-going radiant heat flux along the vector normal to the flame surface. In this work, the flame surface is predicted with the criterion

$$\left|\tilde{Y}_{s}+\tilde{Y}_{rq}\right| \leq C_{SF} \frac{Y_{O_{s}}^{0}}{s}$$

$$(4.29)$$

where C_{sF} is an empirical constant. It is believed that this positive C_{sF} would influence the number of cells which are involved in the averaging process, but it would not hugely influence the value of the averaged variable, such as radiant heat flux, over the flame surface. The unit vector normal to the flame surface (\hat{n}_{sF}) may be expressed using the gradient of the reference species and soot mass fraction:

$$\hat{n}_{SF} = -\frac{\nabla \left(\tilde{Y}_{s} + \tilde{Y}_{ref}\right)}{\left|\nabla \left(\tilde{Y}_{s} + \tilde{Y}_{ref}\right)\right|}$$
(4.30)

According to Eq. (4.8), the local out-going radiant heat flux along the vector normal to the flame surface (q_{SF}^{*}) would be written as

$$q_{SF}'' = \int_{\hat{s} \cdot \hat{n}_{SF} > 0} I(\boldsymbol{x}, \hat{s})(\hat{s} \cdot \hat{n}_{SF}) d\Omega$$
(4.31)

Hence, the surface emissive power on the flame surface (SEP_{SF}) could be expressed as

$$SEP_{SF} = \frac{\sum_{cell} q_{SF,cell}^* dV_{cell}}{\sum_{cell} dV_{cell}} \bigg|_{|\hat{Y}_{c} + \hat{V}_{rel}| \leq C_{SF}} \frac{Y_{0,c}^{0}}{\epsilon}}{\epsilon}$$
(4.32)

Note that the surface area weight is preferred to average the surface emissive power, and here the volume weight is adopted instead in order to bypass the wrong prediction of surface area, as described earlier.

4.4.3 Surface Emissivity

In this method, the surface emissive power would be estimated from the local emissivity over the flame surface. The local flame emissivity (e_{Δ}) may be estimated as

$$e_{\Delta} = 1 - \exp(-\kappa\Delta) \tag{4.33}$$

Note that here the filter width is applied to represent the typical beam length in each cell. The local surface emissive power (SEP_A) may be expressed as

$$SEP_{\Delta} = e_{\Delta}\sigma\tilde{T}^{4} \tag{4.34}$$

Therefore, the surface emissive power over the flame surface would be

$$SEP_{SF} = \frac{\sum_{cell} SEP_{\Delta,cell} dV_{cell}}{\sum_{cell} dV_{cell}} \bigg|_{\dot{Y}, \dot{Y}_{rel} \mid SC_{SP}} \frac{Y_{O_{T}}^{n}}{s}$$
(4.35)

It is noted that the criterion Eq. (4.29) is still used here to representatively capture the flame surface.

Chapter 5

FireFOAM Solver

5.1 INTRODUCTION

FireFOAM, a fully compressible LES solver for buoyancy driven flows and diffusion combustion, is based on the OpenFOAM platform [110], which is a set of object-oriented open source CFD toolboxes written in C++. Based on the conservative finite volume method, the code can even use unstructured polyhedral mesh, and it also benefits from parallelization. The use of the objectoriented programming technique makes it possible to avoid the recompilation of the overall source code. After changing part of the code, through the concept of dynamic library the unchanged part can just be called upon directly to link with any newly developed models.

FireFOAM has benefitted from both contract supported development as well as internal development by FM Global. The long term goal of FireFOAM is the predictive capability of large scale industrial fires and water based suppressions [5]. Relevant mathematical models, such as surface film model, pyrolysis model and suppression model, are currently on-going at FM Global. The present study is merely focused on the development of robust combustion and soot model. The basic governing equations, discretization method, and iteration technique are included in the following sections.
5.2 GOVERNING EQUATIONS

The governing equations are expressed as follows. The over-bars and tildes stand for spatial filtering and Favre averaging in the LES framework, respectively.

<u>Mass</u>

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_{j}}{\partial x_{j}} = 0$$
(5.1)

Momentum

$$\frac{\partial \bar{\rho} \bar{u}_{i}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_{i} \bar{u}_{j}}{\partial x_{j}} = -\frac{\partial \bar{p}}{\partial x_{i}} + \frac{\partial}{\partial x_{j}} \left(\bar{\rho} \left(v + v_{i} \right) \left(\frac{\partial \bar{u}_{i}}{\partial x_{j}} + \frac{\partial \bar{u}_{j}}{\partial x_{i}} - \frac{2}{3} \frac{\partial \bar{u}_{k}}{\partial x_{k}} \delta_{ij} \right) \right) + \bar{\rho} g_{i}, \qquad (5.2)$$

$$(i, j, k = 1, 2, 3)$$

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$
(5.3)

Gas Species

$$\frac{\partial \overline{\rho} \tilde{Y}_{m}}{\partial t} + \frac{\partial \overline{\rho} \tilde{u}_{j} \tilde{Y}_{m}}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left(\overline{\rho} \left(D + \frac{v_{i}}{Sc_{i}} \right) \frac{\partial \tilde{Y}_{m}}{\partial x_{j}} \right) + \overline{\omega}_{m,g} + \overline{\omega}_{m,sf} + \overline{\omega}_{m,so}, \qquad (5.4)$$
$$\left(m = fu_{i}, O_{2}, CO_{2}, H_{2}O \right)$$

<u>Soot</u>

$$\frac{\partial \overline{\rho} \tilde{Y}_{s}}{\partial t} + \frac{\partial \overline{\rho} \tilde{u}_{j} \tilde{Y}_{s}}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left(\overline{\rho} \left(D_{s} + \frac{v_{t}}{Sc_{t}} \right) \frac{\partial \tilde{Y}_{s}}{\partial x_{j}} \right) + \overline{\omega}_{s,f} + \overline{\omega}_{s,o}$$
(5.5)

Sensible Enthalpy

$$\frac{\partial \bar{\rho} \tilde{h}_{s}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_{j} \tilde{h}_{s}}{\partial x_{j}} = \frac{D \bar{p}}{D t} + \frac{\partial}{\partial x_{j}} \left(\bar{\rho} \left(\alpha + \frac{v_{t}}{P r_{t}} \right) \frac{\partial \tilde{h}_{s}}{\partial x_{j}} \right) + \dot{q}'' - \nabla \cdot \dot{q}_{r}''$$
(5.6)

$$\tilde{h}_{s} = \int_{T_{0}}^{\tilde{\tau}} \sum_{m} \left(C p_{m}(\tau) \tilde{Y}_{m} \right) d\tau$$
(5.7)

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$$\frac{Dp}{Dt} = \frac{\partial p}{\partial t} + u \cdot \nabla p \tag{5.8}$$

$$\dot{q}^{\prime\prime\prime} = \omega_{f_{\rm u},g} \Delta h_c - \omega_{s,o} \Delta h_{c,s} \tag{5.9}$$

Equation of State

$$\overline{p} = \overline{\rho} \frac{R}{MW_{ave}} \tilde{T}$$
(5.10)

$$\frac{1}{MW_{ave}} = \sum_{m} \left(\frac{\tilde{Y}_{m}}{MW_{m}} \right)$$
(5.11)

It is worth pointing out that the relevant source/sink terms in Eqs. (5.4), (5.5), and (5.9) have already been described in detail in the "combustion model" and "soot model" sections.

5.2.1 LES Model

The goal of LES model is to represent the SGS stress in terms of resolved velocity field and meanwhile to estimate the turbulent viscosity. The most popular model is the algebraic eddy viscosity model originally proposed by Smagorinsky [23]. However, this model is not capable of coupling with EDC as the SGS kinetic energy cannot be obtained, which is the essential variable to apply the newly developed EDC to LES as mentioned before. From this point of view, the one-equation eddy viscosity LES model of Menon et al [23] is a good choice, as it would solve the SGS kinetic energy directly unlike the majority of LES models and meanwhile maintain the simplicity. This model is utilized in the current work, written as

$$\frac{\partial k_{SGS}}{\partial t} + \frac{\partial \tilde{u}_j k_{SGS}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{v_i}{\Pr_i} \frac{\partial k_{SGS}}{\partial x_j} \right) - \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - \varepsilon_{SGS}$$
(5.12)

$$\varepsilon_{SGS} = C_{\varepsilon} \frac{k_{SGS}^{3/2}}{\Delta}$$
(5.13)

$$v_t = C_t k_{SGS}^{V2} \Delta \tag{5.14}$$

$$\tau_{ij} = -2\nu_i \overline{S}_{ij} + \frac{2}{3} k_{SGS} \delta_{ij}$$
(5.15)

$$\overline{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$
(5.16)

Additionally, this model allows even larger mesh size in comparison with the Smagorinsky model, as the turbulent viscosity is calculated from the SGS kinetic energy solved in each cell, rather than from the resolved strain rate.

5.2.2 Pressure Treatment

The pressure could be decomposed into two parts, including the hydraulic pressure (ρ_{gh}) and the remaining part of pressure (p_{egh}), written as

$$p = p_{\rho gh} + \rho gh \tag{5.17}$$

This treatment facilitates the settings of outlet and open boundary conditions with regard to pressure and velocity. Theoretically, the pressure in Eq. (5.6) and Eq. (5.10) could be replaced by the background pressure, like the procedure in FDS [48], to filter out the effect of sound waves, as fire behaviours generally follow the low Mach number assumption [48]. However, FireFOAM still maintains its original format of pressure. As a result, it is not restricted to the low Mach number flows.

As FireFOAM is a fully compressible solver, the treatment of boundary conditions for velocity and pressure should be considered very carefully. In some cases, the distributions of velocity and pressure are found to be non-physical due to the inclusion of sound wave, even though the flow is at a relatively low speed. In fact, we experienced this dilemma in the liquefied natural gas (LNG) fire simulations when there is a cross wind, which is covered in the following sections. At the beginning of simulations, the incoming wind would push the stagnant air, giving rise to the compressible effect and further influencing predictions of pressure and velocity hugely. Attempt was made to pre-define the initial velocity field for the entire internal domain, but the problem persisted. An appropriate boundary condition needs to be developed to handle the outlet boundary in these cases.

It was found that Dp/Dt term in Eq. (5.6) plays a very important role in causing the non-physical enthalpy increase at some locations, resulting in the wrong predictions of temperature, density and velocity. Since Dp/Dt term is believed to be marginal if cross wind is at a low speed, it was decided to neglect this term in such scenarios, but the pressure terms in Eq. (5.2) and Eq. (5.10) are kept the same. This treatment is similar to the low Mach number assumption.

5.3 DISCRETIZATION AND ITERATION

The finite volume method is introduced to discretize these above governing equations. The FVM uses Gauss divergence theorem, which transforms the integrals over a control volume to the integrals over the entire bounding surfaces of the control volume. OpenFOAM provides a lot of options for the discretization of time derivative, convection term, diffusion term, source term, and gradient term, as elaborated in Ref. [111]. In the current work, the time derivative is discretized using the backward time scheme with second order accuracy, and the central differencing scheme with second order accuracy is utilized to discretize both the diffusion term and gradient term. The convection term is discretized using the limited central differencing scheme in order to maintain the total variation diminishing (TVD) characteristic. For the source term, the implicit scheme is adopted.

The PIMPLE algorithm, which is a combination of pressure implicit with splitting of operators (PISO) [112] and semi-implicit methods for pressure-linked equations (SIMPLE) [113], is adopted to update the field variables. There is an inner loop and outer loop in this algorithm, as summarized in Fig. 5.1. The number of these two loops should be specified before the simulation to ensure the numerical solution for all the discretized equations is found. In the outer loop, the momentum equation would be solved firstly with the presumed pressure field (at the last time step), and then the velocity field would be updated. Based on this new velocity field, the gas species equation coupled with our developed EDC in the LES framework, the sensible enthalpy equation imbedded with the effect of soot oxidation on heat transport, and the soot equation implemented with our developed soot formation and oxidation models in LES would be solved and meanwhile the corresponding scalar variables would be updated. As the presumed pressure field has been used in the momentum equation, it is most likely that the continuity cannot stand, and the pressure correction should thus be essential. Note that this correction equation can be derived from the mass and momentum equation, and it is solved in the inner loop of PIMPLE, as shown in Fig. 5.1.

In fact, the above algorithm is very suitable for the incompressible flows, in which there is no pressure equation. In contrast, the equation of state must be included in compressible flows, resulting in the relationship between the pressure,

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density, and temperature. Theoretically, it is not essential to employ PIMPLE to update the pressure, as the pressure could be estimated from the density (continuity equation) and temperature (energy equation). This procedure might be helpful to reduce the numerical cost, since Poisson equation would not be solved. However, the estimated pressure from the density and temperature would vary hugely if they are still not converged, leading to non-physical predictions of the velocity and temperature. The introduction of PIMPLE is expected to enhance the numerical convergence.



Fig. 5.1 The schematic algorithm of the modified FireFOAM solver

5.4 OTHER TREATMENTS

5.4.1 Flame Height

As mentioned in the above section, the whole flame may be captured using Eq. (4.22) for both sooty and non-sooty flames. Hence, the flame height would be

$$L_f = \max\left(\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{g}}\right)|_{\hat{\boldsymbol{y}} + \hat{\boldsymbol{y}} \ge 0}$$
(5.18)

where \hat{x} is a vector representing the coordinate location of cell centre, and \hat{g} is a unit vector indicating the reverse direction of gravity acceleration. The operator "·" represents the inner product of two vectors. It is worth pointing out that the stoichiometric flame height, which is defined only based on the reference species, would be slightly less than the real flame height, as part of soot particles near the flame brink would be oxidized.

5.4.2 Radiative Fraction

The radiative fraction is known as the ratio of radiation loss to the total energy, and it is indeed dependent on the fuel type and pool size. The total radiative fraction over the whole flame (R_r) is calculated from

$$R_{r} = \frac{\sum_{cell} (\nabla \cdot q_{r}^{*})_{cell} dV_{cell}}{\sum_{cell} (\overline{\omega}_{fu,g} \Delta h_{c} + \overline{\omega}_{s,f} \Delta h_{c,s})_{cell} dV_{cell}} \bigg|_{\dot{Y}_{c} + \dot{Y}_{ref} \ge 0}$$
(5.19)

Bear in mind that the energy stored in the soot particles should also be taken into account.

5.4.3 Cross Wind Inlet Boundary

In the large scale LNG fire scenarios, the cross wind speed needs to be considered as the experiments were conducted in a big open area. However, the wind speed is often measured at the relatively lower location during LNG tests, which could not reflect the effect of actual velocity profile on the flame. In order to mimic this effect, the pre-assumed atmospheric velocity profile is applied to the cross wind inlet velocity (u_n) boundary in the current work:

$$u_{in} = u_{in} \left(H_r\right) \frac{\ln\left(\frac{H}{H_0}\right)}{\ln\left(\frac{H_r}{H_0}\right)}$$
(5.20)

where *H* is the height of cell centre on the cross wind boundary. *H*, is the location where velocity was actually measured in the test, while $u_{in}(H_r)$ is the velocity obtained at the location H_r . H_0 is the roughness length, which is generally set as 3 cm [114].

5.4.4 Flame Tilted Angle

As a result of cross wind, the flame would be tilted as described in Fig. 4.2. The total tilted flame angle (θ) from the reverse direction of gravity would be estimated from the averaging of local flame angles (θ_i) over the entire flame envelope:

$$\theta = \frac{\sum_{i} \theta_{i}}{\sum_{i} 1} \Big|_{[\tilde{Y}_{i} + \tilde{Y}_{or}] | SC_{or}} \frac{Y_{o_{2}}^{n}}{s}}$$
(5.21)

In fact, the averaging process is based on the amount of cells located on the flame surface, rather than the volume weight used in SEP and radiative fraction predictions. θ_i would be expressed as

$$\theta_i = \frac{180}{\pi} \arccos\left(\frac{\hat{x}}{|\hat{x}|} \cdot \hat{g}\right)$$
(5.22)

Chapter 6

Small/Medium Scale Pool Fires

6.1 INTRODUCTION

A series of small/medium scale pool fire scenarios are included to test the combustion and soot model aforementioned. A methanol fire would be considered first to verify the combustion model. As methanol flame is totally clean, the soot model is deactivated. Subsequently, other predictions were carried out for methane fires, heptane fire and toluene fire to test the coupled combustion and soot model. In this chapter, the bar over the variable always represents the time averaging rather than the filtering in LES.

6.2 METHANOL FIRE

6.2.1 **Problem Descriptions**

A 30.5 cm diameter methanol pool fire, conducted by Weckman and Strong [115], is considered to test the combustion model. In the experiment, the burner was mounted on a traversing stand that allows radial and axial traverses of the fire flow field to obtain velocity and temperature measurements from the centreline to the edge of the fire. On this basis, a cylindrical computational domain with the size of 180 cm in diameter, 180 cm in height was set to ensure that influence of the outflow boundaries is negligible, as shown in Fig. 6.1. Nonuniform meshes were employed with grid points clustered around the burner

centre and their size gradually increased in the radial and vertical directions, as displayed in Fig. 6.2. Four different grid resolutions were applied to the domain. denoted as "Super-fine", "Fine", "Medium", and "Coarse". The number of cells across the burner was selected to be 96, 72, 48 and 24 accordingly in each of the four meshes. It is worth pointing out that the "Medium" mesh considered here is already finer than that used in the finest resolution case by Wen et al. [116] for the same scenario. Two types of boundary conditions shown in Fig. 6.1 were used in the calculations: free boundary conditions on the surface of the open domain and prescribed mass flow rate profiles at the fuel exit surface. The methanol feeding rate is 1.069 g/s giving a heat release rate of 22.6 kW. The inlet temperature is 338 K, equivalent to the boiling point of fuel methanol. Sub-grid kinetic energy equation was solved with two coefficients set to be $C_k = 0.05$ [23] and $C_{\epsilon} = 0.4$, which are regarded as the default ones for LES model in all following fire scenarios. Note that the setting of C_{e} would be discussed on the basis of turbulent energy cascade in EDC, as included in the following subsection. The turbulent Prandtl number was set to 0.5 according to the corresponding experimental work [115]. Lewis number was set to unity, implying that the thermal diffusivity is equivalent to the mass diffusivity, and this setting is applicable to all following fire scenarios. The integral length scale is calculated to be 0.22 m based on Eq. (2.28). Radiative heat loss was accounted for with the assumption of an optically thin flame. The physical time was chosen to be 20 s to ensure the flame is fully developed. All the above settings are summarized in Table 6.1.



Fig. 6.1 Schematic of the domain for the methanol fire



Fig. 6.2 Schematic of non-uniform meshes for the methanol fire

Table 6.1 Summary of numerical settings for the methanol fire

Experimentalist	Weckman		
Fuel	Methanol		
Fire Size	30.5 cm		
Mass Flow Rate	1.069 g/s		
Theoretical HRR	22.6 kW		
Inlet Temperature	338 K (boiling point)		
Computational Domain	1.8 m (D) × 1.8 m (H)		
Mesh	Non-uniform grids; Cells across burner: Coarse, 24; Medium, 48; Fine, 72; Super-fine, 96		

LES Model	Sub-grid kinetic energy equation $C_e = 0.4$ $C_k = 0.05$		
Radiation Model	Optically thin assumption		
Soot Model	Off		
Prandtl Number	0.5		
Lewis Number	1.0		
Integral Length Scale	0.22 m		
Physical Time	20 s		

6.2.2 Results and Discussions

a. C_{EDC} Term

To some extent, the term C_{EXC} in Eq. (2.20) represents how fast the reaction rate of fuel is consumed during the combustion, and its distribution is described in Fig. 6.3 with γ and χ ranging from 0 to close to 1. It is seen that the value of C_{EXC} increases with the increase of γ and χ . The values are almost two orders of magnitudes greater when γ and χ are close to 1, reflecting the possible big change in different cells due to the variation of γ and χ . According to the appearance of C_{EXC} in Eq. (2.20), one may think about the similarity between C_{EXC} and the coefficient " λ " in the eddy dissipation model [6]. It is described in [6] that " λ " may depend on the structure of flame, but generally it is set as 4. Bilger [11] suggested that this coefficient may be computed explicitly as a function of the mixture fraction mean and standard deviation, and that it is not strongly dependent on the shape of the commonly used mixture fraction PDF. In this study, C_{EXC} is determined by both the turbulence (in γ) and composition (in χ).



Fig. 6.3 C_{EX} as a function γ and χ

b. Grid Sensitivity

The effect of grid size on the simulation results is examined to ensure that the grid size is appropriate. In this subsection, both the mean and fluctuation properties would be checked with the variation of the grid size. The mean centreline temperature rise and centreline axial velocity are firstly considered, as shown in Figs. 6.4 and 6.5. These two variables could represent the effect in the whole domain. The empirical model developed by McCaffrey [117], which is widely used in the fire community, is also introduced:

$$\frac{u_z}{Q^{3/5}} = A \left(\frac{z}{Q^{2/5}}\right)^{\eta} \tag{6.1}$$

$$\frac{2g\Delta T}{T_{\infty}} = \left(\frac{A}{B}\right)^2 \left(\frac{z}{Q^{2/5}}\right)^{2\eta-1}$$
(6.2)

The coefficients for this model are summarized in Table 6.2. It is worth pointing out that three zones, including "flame" zone $(\frac{z}{Q^{2/5}} < 0.08)$, "intermittent" zone $(0.08 \le \frac{z}{Q^{2/5}} \le 0.2)$, and "plume" zone $(\frac{z}{Q^{2/5}} > 0.2)$, are considered in this model, where the different value would be specified for each coefficient. It is also worth mentioning that the properties in this experiment are measured under the height of 30 cm, i.e. $\frac{z}{Q^{2/5}} = 0.086$, indicating that the measurement would be majorly located in the "flame" zone.

A	В	η	$z/Q^{2/5}$ (m/k $W^{2/5}$)
6.8 m ^{1/2} /s	0.9	1/2	<0.08
1.9 m/s/kW ^{1/5}	0.9	0	0.08-0.2
1.1 m ^{4/3} /s/kW ^{1/3}	0.9	-1/3	>0.2
	A 6.8 m ^{1/2} /s 1.9 m/s/kW ^{1/5} 1.1 m ^{4/3} /s/kW ^{1/3}	A B $6.8 \text{ m}^{1/2}/\text{s}$ 0.9 $1.9 \text{ m/s/kW}^{1/5}$ 0.9 $1.1 \text{ m}^{4/3}/\text{s/kW}^{1/3}$ 0.9	A B η $6.8 \text{ m}^{1/2}/\text{s}$ 0.9 $1/2$ $1.9 \text{ m/s/kW}^{1/5}$ 0.9 0 $1.1 \text{ m}^{4/3}/\text{s/kW}^{1/3}$ 0.9 $-1/3$

Table 6.2 McCaffrey model coefficients

In Fig. 6.4, it is found that the measurement is around 200 K higher than the empirical McCaffrey model in the "flame" zone, while it would follow the trend of that model near the start of the "intermittent" zone. The "Coarse" simulation surprisingly achieved good agreement with the measurement at the beginning of "flame" zone, while the discrepancy became larger and larger starting from $\frac{z}{Q^{2/3}} = 0.05$. One can also find that the predicted temperature would decrease with the increase of grid resolution. This finding is thought to be relevant to the foundation of EDC. It is known that in EDC the reaction rate is formulated based on the turbulent properties, and thus the resolution of turbulence would have a big impact on the reaction rate. In Eqs. (2.20) and (2.22), one can derive that the reaction rate would decrease with the decrease of the total dissipation rate. Moreover, in this study the total dissipation rate is modelled in terms of SGS kinetic energy, as shown in Eq. (2.12). Theoretically SGS kinetic energy represents the cut energy because of the filtering process, and it would decrease when the filtered width estimate from the cubic root of the cell volume decreases. Therefore, it is most likely that the reaction rate would decrease with the increase of grid resolutions.

The "Medium" and "Fine" meshes give similar predictions, while the prediction of the "Super-fine" mesh deviates from both curves. This is possibly explained by the fact that the grid size (3.2 mm) on the burner is quite close to the Kolmogorov length scale, as shown in Fig. 6.32. Hence the simulation using the "Super-fine" mesh would be similar to direct numerical simulation (DNS). As the SGS kinetic energy is expected to be really small when the filter width is very close to the Kolmogorov length scale, it may influence the credibility of the total dissipation rate ε as well as the mass transfer rate between fine structures and surrounding fluid, i.e. \dot{m} " in Eq. (2.22).



Fig. 6.4 Centerline temperature rise as a function of normalized height

Figure 6.5 describes the normalized centreline axial velocity $\left(\frac{u_z}{O^{1/5}}\right)$ as a

function of the normalized height $(\frac{z}{Q^{V3}})$. As one can see, there is considerable difference between the measurement and McCaffrey empirical model in the "flame" zone, although they appear to follow a similar trend. Overall, the "Coarse" mesh over-predicts the velocity in all three zones. In contrast, "Medium", "Fine" and "Sup-fine" meshes achieves the reasonable agreement with the measurement in the "flame" zone. One can also find the predictions with those three meshes peak in the "intermittent" zone similar to McCaffrey's correlation, while they deviate from the empirical curve in the "plume" zone. As to this deviation, it would be unfair to say the current predictions are bad, since there is no corresponding experimental data. The deviation is also likely due to the differing stoichiometries of the fuels as McCaffrey's correlation was developed based on the methane fires.



Fig. 6.5 The normalized centerline axial velocity as a function of normalized

height

Comparison of the predicted temperature fluctuation $\overline{T'}$ and Reynolds stress $\overline{u'_{i}u'_{i}}$ (radial direction and axial direction) with different meshes are made in Fig. 6.6 and Fig. 6.7, respectively. It is found that the "Coarse" mesh underpredicts both $\overline{T'}$ and $\overline{u'_{i}u'_{i}}$, while the "Medium" and "Fine" meshes give very similar results, indicating that the medium grid resolution should be sufficiently fine. One can also observe that the predictions with the "Medium" and "Fine" mesh are in reasonable agreement with the experimental data.



Fig. 6.6 Comparison of the temperature fluctuation $\overline{T'}$ ((a)---coarse mesh; (b)--medium mesh; (c)---fine mesh; (d)---experiment)



Fig. 6.7 Comparison of Reynolds stress $\overline{u'_x u'_z}$ ((a)---coarse mesh; (b)---medium mesh; (c)---fine mesh; (d)---experiment)

c. Effect of New γ

The mass fraction occupied by the fine structures, i.e. γ , is obtained based on Eq. (2.28), as described in Chapter 2. Note that the integral length scale formula is applied. The predicted transient (at 20 s) and average distribution of γ is illustrated in Fig. 6.8. It is found in the transient profile that the magnitude of γ ranges from 0.25 to 0.5. The greater values are generally located near the fire base, particularly close to the two side open boundaries. It is also evident in the average profile. As a matter of fact, γ would be only dependent on the total dissipation rate ε if the integral length scale L' is pre-described, according to Eq. (2.27), and it could be expressed as

$$\gamma \propto \varepsilon^{(D-3)/4} \tag{6.3}$$

As *D* is less than 3, γ would decrease with the increase of ε , and one can also find this trend by comparing with Fig. 6.8 and Fig. 6.27.



Fig. 6.8 Calculated transient and average distributions of γ with the introduction

d. Effect of New X

Two cases are designed in order to understand the effect of χ , and the only difference is the expression of χ , either the original expression of Eq. (2.33)

or the newly developed expression of Eq. (2.47). The calculated transient (randomly chosen at 20 s) and average distributions of χ and T across the burner centre using Eq. (2.33) are shown in Fig. 6.9. For the transient χ , it seems to be unreasonable that the value of χ near the fire source is close to 0, while it is around 1 in the non-reaction areas. Actually, \tilde{Y}_{ρ} term in Eq. (2.33) tends to remain 0 near the burner exit, which is due to the fact that no combustion will take place if the small value is not added to χ initially, causing the chemical reaction to be frozen in this area. In contrast, \tilde{Y}_{μ} term would become 0 in the far field, and the calculated value of χ will be 1 as long as \tilde{Y}_{ρ} is not equal to 0. In the transient T profile, weak temperature increase is found near the burner exit and the flame is surprisingly lifted from the burner, which is non-physical for a pool fire. The possible reason is due to the unreasonable distribution of χ .

Regarding the average χ , its magnitude increases with the height along the centreline, and χ distribution generally could not represent the flame structure. The non-physical lifted flame is also evident in the average T profile. It is also shown that the magnitude of predicted average T is much smaller than the transient one in the lifted reaction area, implicitly reflecting that the lifted reaction area was on the move. Moreover, this movement may be the reason why there is another relatively high temperature core in the far field of average Tprofile.



Fig. 6.9 Calculated transient and average distributions of χ and T using Eq. (2.33)

Figure 6.10 describes the calculated transient and average χ and T with the new expression, i.e. Eq. (2.47). It is indicated that the larger value of χ occurs where the flame temperature is predicted to be higher, implying that the larger reaction rate gives rise to the higher temperature according to the relationship between C_{exc} and χ . In fact, this is the fundamental basis of the proposed modification. Unlike the above predictions with the original expression of Eq. (2.33), the flame is anchored to the burner which is consistent with experimental observations [115]. Furthermore, the average T distribution appears to agree with the common temperature profile for pool fires [109], and the detailed comparison would be made in the below subsection.



Fig. 6.10 Calculated transient and average distributions of χ and *T* using Eq. (2.47) e. Effect of Initial Conditions on χ

With regard to the previous predictions using the original expression of Eq. (2.33), one might argue that the settings of initial conditions may be inappropriate, and think that the ignition process must be employed if the

original expression is activated. Here three cases are designed with the different ignition method or different size of ignition region, and bear in mind that all these cases are performed using the original express of χ .

The first method for ignition would be using relatively high temperature. In this case, the ignition temperature of 1000 K is initially applied to the region with 0.5 m \times 0.5 m \times 0.5 m on the top of the burner. The physical time is set as 20 s, the same value as before. The predicted transient (at 20 s) and average distributions of χ and T are included in Fig. 6.11. It is clear that the predicted transient χ has the similar structure to the one in Fig. 6.9, which is unreasonable based on the previous analysis. Similarly the flame is also believed to be lifted, as the temperature increase near the burner is so weak, evident in the transient and average temperature profile. It is also found that the inclusion of ignition process using high temperature indeed influences the average distributions of χ and T, by comparing Fig. 6.11 with Fig. 6.9. However, this high temperature ignition method couldn't solve the lifted problem.



Fig. 6.11 Calculated transient and average distributions of χ and T using Eq. (2.33) (Ignition method: high temperature; Physical time: 20 s)

Moreover, one may also question whether the physical time is long enough to include all the physical phenomena and to support the above findings. Thus, we continued to run this case up to 100 s in order to clarify the doubt. Fig. 6.12 depicts the predicted transient distributions of χ and T at 100 s, and the nonphysical lifted flame is still there.



Fig. 6.12 Calculated transient distributions of χ and T using Eq. (2.33)

(Ignition method: high temperature; Physical time: 100 s)

The second ignition method applied in this work is the pre-described \tilde{Y}_{pr} , composed of \tilde{Y}_{CO_2} and \tilde{Y}_{H_2O} . Initially, the species mass fractions of CO₂ and H₂O are both set as a constant of 0.5 within the region of 0.5 m × 0.5 m × 0.5 m on the top of the burner, as designed in the previous case. In contrast, the species mass fractions of O₂ and N₂ are both selected to be 0 in that region, leading to $\tilde{Y}_{pr} = 1$ for Eq. (2.33) at the start. The physical time is also chosen as 20 s. The predicted transient (at 20 s) and average distributions of χ and T are presented in Fig. 6.13. The unreasonable distribution of χ and non-physical lifted phenomenon are also evident here, as analysed before. It is also demonstrated that the inclusion of ignition process has some effect on the average distributions of χ and T, in comparison with Fig. 6.9, but cannot really tackle the lifted problem.



Fig. 6.13 Calculated transient and average distributions of χ and T using Eq. (2.33) (Ignition method: pre-described \tilde{Y}_{p} ; Ignition region: 0.5 m × 0.5 m × 0.5 m;

Physical time: 20 s)

For this ignition method, another case is included here to determine if the size of ignition region affects the distributions. In this case, the ignition region is reduced to $0.15 \text{ m} \times 0.15 \text{ m} \times 0.15 \text{ m}$ based on the previous case, and the injected methanol from the burner due to diffusion and convection would have more opportunities to mix with the air at the beginning of the simulation. It is

illustrated in Fig. 6.14 that the unreasonable χ and the lifted problem still exist. Note that the size of ignition region would have an impact on the average χ and T, but still couldn't really improve the weak temperature increase near the burner. The physical time is also prolonged to 100 s to check the possible improvement, but unfortunately the problems are still there, as shown in Fig. 6.15.



Fig. 6.14 Calculated transient and average distributions of χ and T using Eq. (2.33) (Ignition method: pre-described \tilde{Y}_{pr} ; Ignition region: 0.15 m × 0.15 m × 0.15 m;

Physical time: 20 s)



Fig. 6.15 Calculated transient distributions of χ and T using Eq. (2.33) (Ignition method: pre-described $\tilde{Y}_{\rho r}$; Ignition region: 0.15 m × 0.15 m × 0.15 m;

Physical time: 100 s)

f. Heat Release Rate

The predicted curves of heat release rate versus time achieved from different simulations are displayed in Fig. 6.16. Before analyzing those curves, it is worth mentioning that in the following discussions the predictions simulated using not only the new expression of χ but also the original one would be considered, in order to further investigate the possible improvement due to this new expression. In the above analysis, three different approaches, including "no ignition method", "the high temperature ignition method" and "the pre-described $\bar{Y}_{,r}$ ignition method", have already been included when the original expression is applied, but the prediction with the high temperature ignition method would be chosen arbitrarily to represent the results. It is already proved that all those three approaches could not resolve the lifted problem fundamentally, and that choice to display the results would thus be insignificant. For convenience, the prediction obtained from the new expression of χ is denoted as "new" for this scenario, while the one from the original expression coupled with the high temperature ignition method is referred to as "original".

It is found in Fig. 6.16 that both "new" and "original" predictions show the character of oscillation. This must be associated with the periodic vortex shedding in the pool fire [118]. However, the predicted oscillation period is so distinct due to the expression of χ . The calculated period in the "original" simulation would be around 2.5 s, approximately 6 times larger than the one in the "new" simulation. According to [118], this magnitude is totally non-physical. It is very likely that the lifted problem, as illustrated before, has influenced the flame puffing behaviour of being a pool fire.

Conservation of energy is also examined in order to ensure that the corresponding inlet boundary conditions are feasible. Meanwhile, it is also helpful to check if the unexpected heat loss due to the numerical models or methods is considerable or not. It is worth pointing out that the heat would be released only from the fuel gas combustion, as the soot model is deactivated for this methanol fire. In this situation, the time-averaged heat release rate Q would be equivalent to the total energy Q_i , according to Eq. (3.37). Note that the quasisteady state would be essential to make that equivalence reasonable, and in this work the period from 5 s to 20 s is assumed to be in that state. After averaging those oscillated curves in Fig. 6.16, the magnitude of heat release rate predicted in the "new" simulation would be 22.5 kW, which is very close to the theoretical value, i.e. 22.6 kW. In contrast, the value achieved from the "original" simulation would be 17.5 kW, and thus there is about 25.8 % unexpected heat loss, demonstrating the poor quality regarding the conservation of energy.



Fig. 6.16 The predicted heat release rate versus time for simulations with the new or original expression of χ

g. Flame Height

The predicted flame height as a function of time for the "new" and "original" simulations is shown in Fig. 6.17. It is also clear that the characteristic oscillation of flame height is changed because of employing the original expression of χ . It is already known that the periodic variation of flame height is caused by the movement of large eddies initially formed near the burner rim [119]. These eddies would grow bigger with the increase of height, and meanwhile squeeze the flame from two different sides, resulting in the short neck approximately at the height of one diameter [116]. Finally the flame would break up downwards. Based on the fact that the flame is predicted to be lifted in the "original" simulation, the above mechanism becomes more fragile, as the formation of eddies is limited at the burner rim because of the weak air entrainment. This could be the fundamental reason why the original expression of χ predicted the unreasonable puffing behaviour.

The mean flame height in the "original" simulation is predicted to be 0.58 m, which is around 75 % larger than the one in the "new" simulation, i.e. 0.33 m. According to the experimental finding [115], the mean flame height may be 0.2 m. Therefore, the new expression of χ further shows its potential, although it may over-predict the flame height. Always bear in mind that the methanol flame is generally in blue, as no soot is formed. Thus, it would be very difficult to distinguish the flame from the environment, leading to the problem to capture its variation of flame height.



Fig. 6.17 The predicted flame height versus time with the new or original

expression of χ

h. Radiative Fraction

As soot model is deactivated for the methanol flame, the gas phase radiation (mainly due to CO_2 and H_2O) would become important. It is previously shown that the gas phase absorption coefficient is obtained from the RADCAL program [104]. Therefore, the radiative fraction could be helpful to examine the feasibility of that program in this scenario. The predicted radiative fraction against time is depicted in Fig. 6.18. For the "new" simulation, the mean radiative fraction is calculated to be 0.19. Unfortunately, this property was not measured during the experiment. In a similar experimental study, Gore [120] obtained the value of 0.18 for a 30 cm methanol fire. Although the burner size is slightly different, at least his study could give us a hint about the magnitude of radiative fraction for this small scale methanol fire. The current prediction agrees very well with this magnitude.

Regarding the "original" simulation, the non-physical oscillation is still evident, and the average radiative fraction is estimated to be 0.05. As a matter of fact, the radiative fraction generally varies from approximately 0.15 for low sooting fuels, such as most alcohols, to 0.60 for high sooting fuels [119]. Therefore, that predicted value is physically unreasonable. One should always remember that the radiative fraction in this study is based on the whole flame, which is identified according to Eq. (4.22). As a result of the lifted problem in the "original" simulation, the whole flame is artificially extended, as evident in Fig. 6.17. Therefore, that predicted radiative fraction, i.e. 0.05 could not reflect the radiative character of the whole flame.



Fig. 6.18 The predicted radiative fraction versus time with the new or original expression of χ

i. Velocity

The mean axial velocity at different locations (6, 10, 18, and 30 cm) is presented in Fig. 6.19. Overall, the agreement between the "new" simulation and the measurement is qualitatively good. In contrast, the "original" simulation hugely underestimates the magnitude of axial velocity, particularly close to the burner. Figures 6.20 and 6.21 represent the comparison between the predicted and measured radial velocity distributions. It can be seen that the "original" simulation under-predicts the radial velocity, especially near the fire base. The reason would be associated with the weak air entrainment due to the lifted problem. It is found that the "new" simulation gives the reasonable agreement with the experimental data. It is also true with regard to the comparison of the predicted Reynolds stress $\overline{u'_iu'_i}$ with the measurement, as shown in Fig. 6.22.


Fig. 6.19 Comparison of the predicted mean axial velocity with the measurements at different heights



Fig. 6.20 Comparison of the predicted mean radial velocity with the measurements at different heights



Fig. 6.21 Comparison of the predicted radial velocity with the measurement ((a)-

--original; (b)---new; (c)---experiment)



Fig. 6.22 Comparison of the predicted Reynolds stress $\overline{u'_{a}u'_{a}}$ with the measurement ((a)---original; (b)---new; (c)---experiment)

j. Temperature

Similarly, a comparison of the mean temperature at different heights is presented in Fig. 6.23. It is shown that the "original" simulation significantly under-predicts the mean temperature at all heights considered. The predicted

temperature rise near the centreline is not considerable at the locations lower than 18 cm, further demonstrating the existence of lifted phenomenon. In the "new" simulation, the prediction follows the similar trend to the measurement. At H=6cm, the temperature is under-predicted by around 250 K near the centreline. This under-prediction is thought to be due to the basis of the EDC. It is known that in EDC the rate of combustion is linked to the predicted level of turbulence. Immediately above the burner surface, the turbulence level is extremely low and the flow could even be laminar. Thus it would influence the capability of EDC model in this area. Furthermore, it is also noted that it is really difficult to fully capture the transition from laminar to turbulence using the current one-equation eddy viscosity LES model, and that the special treatment for the boundary should also be needed. Apparently, this is not the scope of this study. With the increase of height, the predicted temperature by EDC becomes closer to the experimental data. As the height increases, more air is entrained into the flame, and more large eddies are produced. The flow becomes more turbulent due to the eddy break-up, to which EDC would be more suitable.

Figure 6.24 depicts the predicted and measured temperature fluctuation $\overline{T'}$ profiles. For the "new" simulation, the contour lines cluster near the burner rim at radial positions between 12 cm to 16 cm, which is consistent with the experimental finding [115]. The discrepancy from the measurement occurs in the region near the centreline of the pool, as one can find the magnitude of the predicted temperature fluctuations increases gradually along the centreline with the increase of height. For the "original" simulation, the magnitude of the increase of height. For the "original" simulation, the magnitude of the lifted problem.

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Fig. 6.23 Comparison of the predicted mean temperature with the measurements at different heights



Fig. 6.24 Comparison of the predicted temperature fluctuation $\overline{T'}$ with the measurement ((a)---original; (b)---new; (c)---experiment)

k. Turbulent Heat Flux

Comparisons of the predicted turbulent heat flux $\overline{u'_x T'}$ (radial direction) and $\overline{u'_x T'}$ (axial direction) with the measurements are shown in Figs. 6.25 and 6.26. These two variables are calculated from

$$\overline{u_x'T'} = \overline{u_xT} - \overline{u_xT}$$
(6.4)

$$\overline{u_z'T'} = \overline{u_zT} - \overline{u_zT} \tag{6.5}$$

Note that these two formulae are feasible only for the time averaging process, not for the filtering. It is obvious that the "original" simulation significantly underpredicts the turbulent heat flux $\overline{u'_{i}T'}$ in the whole considered area, as a result of the lifted problem. As discussed before, the lifted phenomenon would hugely influence air entrainment of the flame, and thus the radial velocity fluctuation is definitely weakened. Moreover, the weak temperature rise in that area also plays an important role in this unreasonable distribution of $\overline{u'_{i}T'}$. However, this variable is well predicted in the "new" simulation, as both the magnitude and structure are well captured. The turbulent heat flux $\overline{u'_{i}T'}$ is also under-estimated in the "original" simulation. Furthermore, the contour line near the centreline is predicted to be opposite to the measurement. Nevertheless, the "new" simulation provides reasonable agreement with the measurement in terms of magnitude and distribution.



Fig. 6.25 Comparison of the predicted turbulent heat flux $\overline{u'_{x}T'}$ with the measurement ((a)---original; (b)---new; (c)---experiment)



Fig. 6.26 Comparison of the predicted turbulent heat flux $\overline{u'_{\perp}T'}$ with the measurement ((a)---original; (b)---new; (c)---experiment)

I. Dissipation Rate

According to Eq. (2.8) and Eq. (2.10), W_{sGS} is the dominating term in the calculation of total dissipation rate since its magnitude is always larger than $1/3q_{sGS}$ in the turbulent energy cascade. This magnitude difference would be

bigger if the filter width of LES is located closer to the integral length scale and smaller if the filter width is approaching the Kolmogorov length scale. On the last structure level which is assumed to be of the Kolmogorov scales in this study, the ratio of $1/3q_{scs}$ to W_{scs} would become 1/3 due to the energy balance between q_{scs} and W_{scs} . Hence, $1/3q_{scs}$ is expected to play an auxiliary role in the total dissipation rate when LES approaches DNS. Moreover, W_{ses} may be approximated as the SGS dissipation rate ε_{scs} in the sub-grid kinetic energy equation [23] since they have the same expression as a function of k_{scs} and Δ , except the empirical coefficient. In this work, the coefficient C_c in the sub-grid kinetic energy equation, i.e. Eq. (5.13), is modified from 1.0 in [23] to 0.4 according to the term of $(2/3)^{V_2} C_{D_1}$ in W_{scs} expression. Normally LES cannot resolve the scales very close to the Kolmogorov length scale, and there would be little difference between the SGS dissipation rate and the total dissipation rate as evident from the relevant mean distributions in Fig. 6.27. Additionally, the magnitude of the predicted total dissipation rate and SGS dissipation rate in the "original" simulation are generally lower than 20 % of the corresponding one in the "new" simulation.



Fig. 6.27 The predicted mean SGS and total dissipation rate ((a)--- ϵ_{sgs}

,original;(b)--- ε_{sgs} , new; (c)--- ε , original; (d)--- ε , new)

m. Kinetic Energy

The SGS kinetic energy is regarded as an integral of the spectral energy [24] over the wave-numbers from $2\pi/\Delta$ to infinity and indirectly reflects the unresolved velocity fluctuations in LES, while the total kinetic energy is

considered as the integral over all the wave-numbers, i.e. from 0 to infinity, implying the magnitude of instantaneous velocity deviation from the timeaveraged velocity. While the total kinetic energy can be measured during experiments, the SGS kinetic energy only "exists" in models. Generally, the SGS kinetic energy is very small in comparison with the total kinetic energy, as evident in Figs. 6.28 and 6.29.

It is found in Fig. 6.28 that the predicted SGS kinetic energy with the original expression of χ is roughly one tenth of the one with the new expression, further demonstrating the weak turbulence near the burner due to the lifted flame. Bear in mind that this statement is true only if the same filter width is applied in both the "original" and "new" simulations. For the turbulent kinetic energy, it could be derived from the velocity fluctuations and the unresolved SGS kinetic energy, expressed as

$$k_{\text{solal}} = \frac{1}{2} \left(\overline{u'_{x} u'_{x}} + \overline{u'_{y} u'_{y}} + \overline{u'_{z} u'_{z}} \right) + k_{SGS}$$
(6.6)

Comparison of the predicted k_{total} with the measurement indicates the "new" simulation is capable of achieving the reasonable agreement with the experimental data, as shown in Fig. 6.29, while the "original" simulation fails to do so.



Fig. 6.28 Comparison of the predicted SGS kinetic energy ((a)---original; (b)---

new)



Fig. 6.29 Comparison of the predicted turbulent kinetic energy k_{total} with the measurement ((a)---original; (b)---new; (c)---experiment)

n. Time Scales

The integral time scale and Kolmogorov time scale are very important in turbulent flames, reflecting the residence time of largest eddies and small eddies, respectively. As stated in Chapter 3, the geometric mean of these two time scales is employed to account for the turbulent mixing time scale of soot formation. Therefore, it would be essential to ensure that these two scales are reasonably predicted. Comparison of the predicted integral time scale with the measurement is depicted in Fig. 6.30. The predicted integral time scale in the "new" simulation ranges from 1 s to 3 s in the major parts of the considered area, which agrees well with the experimental data. This variable is predicted around two times larger than the measurement in the "original" simulation. Overall, both "new" and "original" simulations could give a reasonable order of magnitude with regard to the integral time scale. It is worth mentioning that the "new" and "original" simulations are designed in order to demonstrate the capability of the new χ expression, and the structure of EDC model is kept the same. Based on the above information, one would realize that the new developed EDC combustion model could deliver the reasonable time scale of largest eddies, which is very encouraging in LES.

The Kolmogorov time scale reflects the residence time of the smallest eddies, where the combustion is expected to take place as molecular diffusion would be dominant rather than the mechanical movement. In this study, the laminar kinematic viscosity v in Kolmogorov time scale formula Eq. (2.17) is estimated from the Sutherland transport equation, expressed as [121]

$$\nu = \frac{A_s \sqrt{T}}{\rho (1 + T_s / T)} \tag{6.7}$$

where A_{i} and T_{i} are applied as 1.67E-6 and 170.67 respectively. With the help of time-averaged temperature and density profiles, one could approximate the distribution of the Kolmogorov time scale, as displayed in Fig. 6.31. It is found that the "original" simulation gives a bit larger value of this time scale than the

one in the "new" simulation, particularly in the intermittent flame. However, the order of magnitude is the same for both simulations, which is predicted to be 10~100 ms. Figure 12 in Ref [115] demonstrated that the experimental data for this time scale is around 30~60 ms at the height of 8 cm, while the prediction is approximately 80 ms, proving that the current extension of EDC could have the potential to deliver the reasonable range of Kolmogorov time scale. As a matter of fact, it is very encouraging indeed, as this time scale is extremely significant for the turbulent combustion simulations.



Fig. 6.30 Comparison of the predicted integral time scale τ_1 (s) with the measurement ((a)---original; (b)---new; (c)---experiment)



Fig. 6.31 Comparison of the predicted Kolmogorov time scale τ_{η} (ms) ((a)---

original; (b)---new)

o. Length Scales

In turbulent flames, there are three popular length scales, including the integral length scale, Taylor length scale and Kolmogorov length scale. As addressed in the Chapter 2, the integral length scale is assumed to be equal to the characteristic plume length in fire dynamics in order to approximate the total kinetic energy as well as the integral time scale. This length scale represents the typical length in the largest eddies where majority of mechanical energy is occupied. As expected, the Kolmogorov length scale determines the typical length of the smallest eddies. The laminar kinematic viscosity in the calculation of this length scale is also obtained from Eq. (6.7) similarly like the estimation of Kolmogorov time scale. The predicted Kolmogorov length scale using the two different expressions of χ is shown in Fig. 6.32. Although the predicted value in the "new" simulation is a bit larger, the order of magnitude for this length scale is

mm in both the "new" and "original" simulations. It is worth pointing out that the Kolmogorov length scale could vary hugely, as it is significantly dependant on the turbulent Reynolds number [24]. The Taylor length scale is somewhere between the integral length scale and the Kolmogorov length scale, which is calculated from Eq. (2.26) in this study. It is found in Fig. 6.33 that the predicted Taylor length scale is on the same order of magnitude, i.e. cm, as the experimental data, demonstrating the capability of the new developed EDC model.

In the experimental work [115], it is found that the ratio of Taylor to Kolmogorov scales is approximately 2.5:1 in the central core of the fire, and increased to 8:1 near the edge of the fire. Based on this relationship, one could work out Kolmogorov length scale should be on the order of magnitude of mm, with the help of measured profile of Taylor length scale in Fig. 6.33. This finding further proves that the predicted Kolmogorov length scale in Fig. 6.32 is in a reasonable range.



Fig. 6.32 Comparison of the predicted Kolmogorov length scale L^{*}(mm) with the measurement ((a)---original; (b)---new)



Fig. 6.33 Comparison of the predicted Taylor length scale λ (cm) with the measurement ((a)---original; (b)---new; (c)---experiment)

p. Comparison with Original RANS-based EDC

In order to further understand possible improvements due to the newly developed LES-based EDC, simulations results of the original RANS-based EDC are included in this paper. Figures 6.34 and 6.35 demonstrate the comparisons of the predicted mean axial velocity and mean temperature using the newly developed LES-based EDC with those utilizing the original RANS-based EDC. It is evident that the original RANS-based EDC significantly under-predicts the mean axial velocity and mean temperature, particularly at the lower locations. It is likely that the existence of the original χ expression plays a dominant role in that under-prediction, as it can result in the weak temperature rise near the burner surface proved in the previous subsection. On the contrary, the predicted mean axial velocity and mean temperature using the newly developed LES-based EDC are in reasonable agreement with the experimental data.



Fig. 6.34 Comparison of the predicted mean axial velocity with the

measurements at different heights



Fig. 6.35 Comparison of the predicted mean temperature with the measurements at different heights

6.3 HEPTANE FIRE

6.3.1 **Problem Descriptions**

A 30 cm diameter heptane pool fire tested by Klassen and Gore [120] is firstly considered for the soot model test. A cylindrical computational domain of 2 m in diameter and 4 m in height was used to minimize the influence of open boundaries, as shown in Fig. 6.36. Non-uniform meshes were employed similarly like the one in Fig. 6.2. Three different meshes were applied to the domain, denoted as "Fine", "Medium", and "Coarse", and the number of cells across the burner is selected to be 72, 48 and 24 accordingly. Three boundary conditions are considered in this scenario including the inlet boundary for the burner surface, the open boundary for the top and sides of the domain, and the wall boundary for the ground, as displayed in Fig. 6.36. The heptane feeding rate is 0.0362 kg/m²s, giving a theoretical heat release rate of 115 kW. The inlet temperature is set as 372 K, equal to the boiling point of heptane. The laminar smoke point height is 0.147 m for fuel heptane [86]. Both turbulent Prandtl number and Schmidt number were set as 0.8. The integral length scale is calculated to be 0.41 m based on Eq. (2.28). FVM with the grey body assumption was activated for the radiation model, which is the default setting for radiative heat transfer. The physical time was chosen to be 20 s to ensure the flame is fully developed. All the above settings are summarized in Table 6.3.



Fig. 6.36 Schematic of the domain for the heptane fire

Table 6.3 Summary	of numerical :	settings for	the heptane	fire

Experimentalist	Klassen and Gore		
Fuel	Heptane		
Smoke Point Height	0.147 m		
Fire Size	30 cm		
Mass Flow Rate	0.0362 kg/m ² s		
Theoretical HRR	115 kW		
Inlet Temperature	372 K (boiling point)		
Computational Domain	2 m (D) × 4 m (H)		
Mesh	Non-uniform grids; Cells across burner: Coarse, 24; Mediun 48; Fine, 72		
LES Model	Sub-grid kinetic energy equation $C_{e} = 0.4$ $C_{k} = 0.05$		
Radiation Model	Finite volume method		
Soot Model	On		
Prandtl Number	0.8		
Lewis Number	1.0		
Integral Length Scale	0.41 m		
Physical Time	20 s		

6.3.2 Results and Discussions

Heptane is a moderately sooty fuel, and thus the soot model is activated in this scenario. Four methods are included here to understand the effect of PaSR, as well as the soot oxidation model. These are denoted as " κ +oxid", "lam+oxid", " κ ", and "lam" in this study. Here " κ " represents the inclusion of PaSR concept, while "lam" means the direct application of the laminar smoke point soot model, i.e. the instantaneous properties being replaced with the filtered ones. Moreover, the sign "oxid" denotes the activation of soot oxidation model, aiming to examine the effect of oxidation model on the flames.

a. Grid Sensitivity

The centreline temperature rise and axial velocity are employed to perform the grid sensitivity studies, as shown in Figs. 6.37 and 6.38. In Fig. 6.37, it is found that the experimental data agrees well with the McCaffrey empirical model in the flame zone and the start of intermittent zone, but the discrepancy is huge in the end of intermittent zone, where $z/Q^{2/5}$ is close to 0.2. Bear in mind that the temperature was measured based on the intensities at two wavelengths [120]. Near the end of intermittent zone, the tested flame intensities may become very weak, and thus the uncertainties of temperature may be larger. The predicted temperature with the "Coarse", "Medium" and "Fine" meshes generally follow the trend of McCaffrey empirical model, and the differences mainly exist in the intermittent zone and plume zone. One could also find that the predicted temperature gets converged when "Medium" and "Fine" meshes are employed, reflecting the independence of the grid resolution. Similarly, the predicted axial velocity is quite close to each other for these "Medium" and

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"Fine" simulations, as shown in Fig. 6.38. Note that the major difference between the predictions and McCaffrey model takes place in the flame zone. Nevertheless, this could not reflect the predictions are not reasonable, as one could also find the similar issue in Fig. 6.5, where the predictions actually perform very well by comparing with the experimental data. Unfortunately, there is lack of the corresponding velocity data in this scenario.



Fig. 6.37 The centerline temperature rise as a function of normalized height



Fig. 6.38 The normalized centerline axial velocity as a function of normalized

height

Comparison of the predicted temperature fluctuation $\overline{T'}$ and turbulent stress $\overline{u'_z u'_z}$ are made in Fig. 6.39 and Fig. 6.40, respectively. As one can see, the "Medium" and "Fine" meshes could deliver very similar temperature fluctuation and turbulent stress $\overline{u'_z u'_z}$ distributions, further supporting the previous statement about the grid independence.



Fig. 6.39 Comparison of the temperature fluctuation $\overline{T'}$ ((a)---coarse mesh; (b)---medium mesh; (c)---fine mesh)



Fig. 6.40 Comparison of the predicted turbulent stress $\overline{u'_z u'_z}$ ((a)---coarse mesh; (b)---medium mesh; (c)---fine mesh)

b. Radiative Properties Sensitivity

The sensitivity study on the radiative properties is conducted, including the number of solid angles and the solving frequency of RTE. Generally, 16 solid angles are used for the discretization of RTE in this study, and RTE is solved and updated every 10 iteration. The number of solid angles was selected to be 16 for radiative transfer equations as a compromise between the computation time and calculation accuracy based on sensitivity studies. Here the solid angles are increased to 64, aiming to understand the effect of solid angle on the radiation. The solving frequency of RTE is also increased to 20 in order to examine whether the radiation source term in the energy equation is updated effectively. The comparison in Fig. 6.41 verifies that those changes of solid angle and solving frequency don't significantly influence the prediction of radiative fraction. Furthermore, this finding makes us confident to utilise the solving frequency of 20 for a series of large scale LNG pool fires, as described later in this Chapter, and thus it could save a lot of computation time.



Fig. 6.41 Comparison of the predicted radiative fraction with the variation of solid angle and solving frequency for RTE

c. Effect of New x

The effect of the new χ expression is also included here. Comparison of the predicted average (20 s for the averaging process) temperature and χ distributions using two different χ expressions is displayed in Fig. 6.42. One could clearly see that the non-physical distribution of χ in the non-reacting area is still existent if the original expression of χ , i.e. Eq. (2.33), is applied, as well as the lifted flame due to the very weak temperature rise near the fuel burner. For the purpose of better checking the lifted problem, the physical simulation time is extended from 20 s to 40 s in case the lifted flame would anchor the burner rim after 20 s. The predicted transient temperature at 40 s with two distinct χ formulae is depicted in Fig. 6.43. It is found that the temperature rise close to the burner is predicted to be 600 K using the original χ expression. As a matter of fact, this temperature is too weak to be regarded inside the flame, as the common flame temperature is more than 1000 K [109]. Therefore, the flame is still lifted evidently. On the contrary, the simulated temperature with the new χ equation of Eq. (2.47) is more than 1000 K in the corresponding area, which agrees well with the common sense of fire dynamics. Actually, the detailed comparison of the predicted temperature with the measurement at different heights and radial positions will be performed in the following subsections. Moreover, the predicted flame width utilizing the original χ equation is much slimmer in comparison with the counterpart. This might be associated with the damage of pool fire mechanism due to the lifted problem.

It is worth mentioning that the initial condition issue considered in the analysis of 30.5 cm methanol fire couldn't apply to this scenario. The main reason is the presence of soot model. Taking the high temperature ignition method as an example, the pre-described temperature rise in one specified region would have a huge impact on the soot formation and oxidation, making the solver very unstable. Therefore, no ignition method is included, and the burning would be automatic as time proceeds, as a consequence of the "mixing-controlled" theory [3].



Fig. 6.42 Calculated average distributions of χ and T with the averaging period of 20 s ((a) and (b)---Eq. (2.33); (c) and (d)---Eq. (2.47))



Fig. 6.43 Comparison of predicted transient temperature at 40 s ((a) ---Eq. (2.33); (b)--- Eq. (2.47))

d. Effect of K

It is known from Eq. (3.15) that κ reflects the relationship between soot chemical time scale ($\tau_{c,s}$) and turbulent mixing time scale (τ_{mix}). Mathematically, if $\tau_{c,s} \ll \tau_{mix}$, $\kappa \rightarrow 0$; if $\tau_{c,s} \gg \tau_{mix}$, $\kappa \rightarrow 1$. Physically, when turbulent mixing time is much longer than soot chemical time scale, soot production would be considered as a fast chemistry process and controlled by the turbulent mixing, and thus soot source term with an Arrhenius-type may not be appropriate. This would correspond to the mathematical analysis of ($\kappa \rightarrow 0$). In contrast, if soot chemical time scale is much longer than turbulent mixing time scale, soot production is expected to occur after the turbulent mixing process, and thus perfect mixing at the sub-grid scale level could be assumed, leading to the possible removal of sub-grid fluctuations [3] in the soot source term. Hence, the instantaneous temperature and fuel mass fraction in Eq. (3.6) could be simply substituted with the filtered properties when extending the original soot model from laminar flames to turbulent flames. This would correspond to the mathematical analysis of $(\kappa \rightarrow 1)$. Soot generation rate would reach its upper limit in this circumstance. Actually, this closure approach is the so-called "lam". Its inclusion is aiming to gain insight about the effect of κ on the predicted soot volume fraction and temperature distributions as discussed in the following subsection, although theoretically it may be inappropriate in most combustion applications [3].

Figure 6.44 depicts the transient and time-averaged κ distribution in the near field of the fire. It is seen that the averaged κ increases vertically with the increase of height up to 5 times the burner diameter while decreases along the radial direction starting from the centreline. The "hump" shape is observed under the height of 1.2 m, which is comparable to the visible flame height of 1.3 m [120], as discussed in the following subsection. This is possibly because the presence of flame surface gives rise to the increase of the predicted SGS kinetic energy and the total dissipation rate, and thus results in the decrease of the turbulent mixing time, as shown in Fig. 6.45. Generally, the magnitude of the transient κ is predicted to be less than 0.5 in the flame area, while this value is slightly greater than 0.5 in the far-field, as a consequence of the relatively strong turbulent mixing. The averaged κ profile suggests that the averaged turbulent mixing time is slightly longer than the fixed soot chemical time scale based on the laminar smoke point height.

In order to further investigate the relationship between the turbulent mixing time scale and soot chemical time scale, the average Kolmogorov time scale, integral time scale, and geometric mean of these time scales are plotted in Fig. 6.45. As one can see, the Kolmogorov time scale generally ranges from

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0.005 s to 0.1 s, while the integral time scale varies from 0.75 s to 4 s in the domain. Correspondingly, the geometric mean of those two time scales is predicted to be from 0.06 s to 1 s, as portrayed in Fig. 6.45. It is known that the soot chemical time scale is calculated to be 0.054 s according to Eq. (3.18), with the smoke point height of fuel heptane, i.e. 0.147 m. Therefore, in this scenario the turbulent mixing time scale would be larger than the soot chemical time scale, but these two time scales are comparable in the majority of the domain. This statement is believed to be consistent with the concept of PaSR, as technically the turbulent mixing process is assumed to proceed after the combustion.



Fig. 6.44 The predicted transient and average κ for PaSR



Fig. 6.45 The predicted average turbulent time scales ((a)---Kolmogorov time scale, s; (b)---integral time scale, s; (c)---geometric mean of Kolmogorov time scale and integral time scale, s)

e. Soot Source Terms

The predicted transient (at 20 s) and average soot formation rate $\omega_{s,f}$ is displayed in Fig. 6.46. The "hump" shape is observed near the fuel burner, which is very much dependent on the temperature distribution. This must be related to the exponential factor of 2.25 for the temperature in the formula of soot formation rate, i.e. Eq. (3.17). In the smoke point concept, the soot formation is assumed to take place only inside the flame, and thus the outline of this rate may represent the flame front. That is the reason why the tip location of the average soot formation rate is consistent with the measured flame height, i.e. 1.31 m.

Figure 6.47 illustrates the transient and average soot oxidation rate $\omega_{x,o}$. It is found that the soot oxidation process takes place outside of the flame but very close to the flame front, and this finding is also evident in the net soot production rate (i.e. $\omega_{x,f} + \omega_{x,o}$) profiles of Fig. 6.48. This is attributed to the limiting conditions in Eq. (3.26). Theoretically in this study the soot oxidation would proceed only if the temperature is high enough and meanwhile the oxygen is relatively rich, inducing the thin oxidation zone. Note that the wide distribution of average $\omega_{x,o}$ must be associated with the turbulent behaviour of the fire. After this oxidation process, the soot particles would be released from the flame, and transport to the far-field due to the convection and turbulent diffusion.



Fig. 6.46 The predicted transient (at 20 s) and average soot formation rate ω_{x}

 $(kg/m^3/s)$



Fig. 6.47 The predicted transient (at 20 s) and average soot oxidation rate $\omega_{s,o}$

 $(kg/m^3/s)$



Fig. 6.48 The predicted transient (at 20 s) and average net soot production rate ω_s in the soot mass fraction transport equation (kg/m³/s)

f. Conservation of Energy

The predicted heat release rate (HRR) and soot potential energy using four different soot model settings, including " κ +oxid", "lam+oxid", " κ ", and "lam", are described in Figs. 6.49 and 6.50. Note that Eq. (3.26) is used for the soot oxidation model here, in which the turbulent mixing time is assumed to be the same as the soot formation.

In Fig. 6.49, it is observed that the inclusion of PaSR has a huge impact on the predicted heat release rate. Actually, the soot volume fraction is 5~10 times over-predicted if the instantaneous temperature and species mass fraction are directly replaced with the corresponding filtered properties in the laminar soot formation term (i.e. "lam"), as discussed in the following subsection. Therefore, a large portion of energy would be stored in the soot particles, of which the component is assumed to be the same as the fuel. This is the reason why "lam+oxid" and "lam" simulations deliver the smaller heat release rate, but the larger soot potential energy, as shown in Figs. 6.49 and 6.50. After applying PaSR, the heat release rate is increased, because some part of energy is artificially released due to the decreased soot volume fraction. One can find the detailed comparison of the predicted soot volume fraction utilizing those four soot model settings with the measurement in Fig. 6.55.

Due to the presence of oxidation model, some part of energy would be released from the soot particles, theoretically giving rise to the larger heat release rate and smaller soot potential energy, in comparison with the simulations without oxidation. This is verified by the slight increase of the amplitude for HRR curves in Fig. 6.49 and the corresponding decrease for soot potential energy curves, provided that the oxidation model is taken into account.

According to the conservation law of energy, the sum of heat release rate and soot potential energy should be kept the same, whatever the soot model settings are applied. This is proved in Fig. 6.51, as one can find all the total energy curves possess the same average value of 115 kW. As a result, it is very close to the theoretical value of 116 kW based on Eq. (3.38), demonstrating the potential of the current models.



Fig. 6.49 The predicted heat release rate with different soot model settings (Eq.

(3.26) for soot oxidation)



Fig. 6.50 The predicted soot potential energy with different soot model settings (Eq. (3.26) for soot oxidation)



Fig. 6.51 The predicted total energy with different soot model settings (Eq. (3.26) for soot oxidation)

g. Flame Height

The predicted flame height with four different soot model settings is described in Fig. 6.52. It appears that the inclusion of PaSR and oxidation model would not have considerable effect on the prediction, although the soot mass fraction would vary a lot as shown in Fig. 6.55, particularly regarding the application of PaSR. The reason is due to the fact that the effect of soot has been accounted for in the formula of flame height, i.e. Eq. (5.18). This method is expected to improve the prediction of flame height in the presence of soot particles, as the soot oxidation zone is also considered. The flame height is calculated to be 1.32 m, which agrees very well with the measurement, i.e. 1.31 m [120].



Fig. 6.52 The predicted flame height with different soot model settings (Eq. (3.26) for soot oxidation)

h. Radiative Fraction

Figure 6.53 demonstrates the predicted radiative fraction in " κ +oxid", "lam+oxid", " κ ", and "lam" simulations. The impact due to the utilization of PaSR is also evident here, as the calculated radiative fractions without PaSR would be smaller than the ones using PaSR. This must be linked to the difference of the predicted soot volume fraction. In fact, the existence of soot particles influences not only the emission, but also the absorption. The oxidation plays a marginal role here. The radiative fraction achieved form the " κ +oxid" simulation is 0.35, in very good agreement with the experimental data, i.e. 0.31 [120].



Fig. 6.53 The predicted radiative fraction with different soot model settings (Eq. (3.26) for soot oxidation)

i. Soot Volume Fraction

The predicted transient and average soot volume fraction contour using " κ +oxid" is described in Fig. 6.54. It is observed that the transient soot volume fraction profile corresponds very well to the transient net soot production rate in Fig. 6.48, and it is predicted to be ranging from 0.4 ~ 2.4 ppm. One could also derive that the soot particles are capable of escaping from the flame, as the soot volume fraction of 0.2 ppm is located above the flame height of 1.3 m in the average profile of Fig. 6.54.

The comprehensive comparison of the predicted mean and root mean square (RMS) of soot volume fraction is performed in Fig. 6.55 and Fig. 6.56 respectively. Note that Eq. (3.25) is used for the soot oxidation in this figure. It can be seen that the "lam" and "lam+oxid" generally over-predict the mean and RMS values 5~10 times in comparison with the measurements [120], demonstrating their poor capabilities in this regard. In contrast, both " κ " and

" κ +oxid" deliver the same order of magnitude as the experimental data. Bear in mind that the soot volume fraction is very small by comparing with the major species, such as CO₂ and H₂O, and the precision of being at the same order of magnitude would be regarded as encouraging. The impact of soot oxidation model is weak at the lower locations, and would enhance with the increase of height, particularly near the rim of the fire plume.

Aiming to gain the insight of that oxidation effect, Eq. (3.26) is also included, which is based on the assumption that the soot formation and oxidation process have the same turbulent mixing time scale. Fig. 6.57 illustrates the comparison of the predicted soot volume fraction and its fluctuation using two different soot oxidation models, i.e. Eq. (3.25) and Eq. (3.26). Note that only " κ +oxid" soot model setting is considered here. It is found that at most locations both two oxidation models are able to give the reasonable agreement with the experimental data. "oxid2", i.e. Eq. (3.25) behaves a bit stronger, as the soot volume fraction and its fluctuation is considerably weakened in the far-field, say H/D=3.4. The reason is due to the application of smallest time scale, i.e. Kolmogorov time scale, to the mixing process after soot oxidation. Eq. (3.26) employs the geometric mean of Kolmogorov time scale and integral time scale as the mixing time scale, leading to the weaker effect as shown in Fig. 6.57. In this study, Eq. (3.26) is preferred, and it will be used in the following simulations, such as methane fires and large scale LNG pool fires.

Additionally, both the predictions and measurements suggest that the magnitude of the RMS soot volume fraction is similar to that of the mean value, indicating that turbulence plays an important role in the instantaneous soot volume fraction distribution in the present case.



Fig. 6.54 The predicted transient and average soot volume fraction (ppm)



Fig. 6.55 The predicted soot volume fraction at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.56 The predicted soot volume fraction fluctuation at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.57 Comparison of the predicted soot volume fraction and its fluctuation using two different oxidation models (oxid1---Eq. (3.26) for soot oxidation;

oxid2---Eq. (3.25) for soot oxidation)

j. Temperature

It is illustrated in Fig. 6.58 that the predicted mean temperature and temperature fluctuations in "lam" and "lam+oxid" simulations are seen to be $0\sim200$ K less than those with " κ " and " κ +oxid". The level of differences is much less than that found in the predictions for soot volume fraction. This is likely because the increase of soot particles does not only increase the radiative emissions but also enhances the absorption, resulting in relatively weak influence of radiation source term on the sensible enthalpy transport equation. Overall, the predicted temperature distributions with the current combustion and soot models are in reasonably good agreement with the measurements. But the predicted

mean temperature profile is slightly wider than the measured profiles at H/D=0.9 and H/D=1.5. The temperature fluctuation is generally under-predicted, as shown in Fig. 6.59. However, the " κ " and " κ +oxid" predictions are believed to be better, as they are more close to the experimental data in comparison with the "lam" and "lam+oxid" results.

The predicted mean temperature and its fluctuation with two different oxidation models, including Eq. (3.25) and Eq. (3.26), are compared in Fig. 6.60 to investigate their impacts. Marginal difference is observed here, as expected. Eq. (3.25) delivers a bit higher mean temperature and its fluctuation due to the fact that more heat is released in the domain as a consequence of the relatively larger oxidation rate.



Fig. 6.58 The predicted temperature at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.59 The predicted temperature fluctuation at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.60 Comparison of the predicted temperature and its fluctuation using two different oxidation models (oxid1---Eq. (3.26) for soot oxidation; oxid2---Eq.

(3.25) for soot oxidation)

6.4 TOLUENE FIRE

6.4.1 Problem Descriptions

A 30 cm diameter toluene pool fire tested by Klassen and Gore [120] is also considered here, and the computational domain and boundary conditions are quite similar to those for the heptane case, as displayed in Fig. 6.36. The toluene feeding rate is 0.0431 kg/m²s with the theoretical heat release rate calculated to be 125 kW. The inlet temperature is set as 384 K, equal to the boiling point of toluene. The laminar smoke point height is 0.008 m for fuel toluene [86]. The integral length scale is calculated to be 0.42 m based on Eq. (2.28). For other settings, this scenario is designed as same as the previous heptane fire scenario, as one can find from Tables 6.3 and 6.4.

Experimentalist	Klassen and Gore				
Fuel	Toluene				
Smoke Point Height	0.008 m				
Fire Size	30 cm				
Mass Flow Rate	0.0431 kg/m ² s				
Theoretical HRR	125 kW				
Inlet Temperature	384 K (boiling point)				
Computational Domain	2 m (D) × 4 m (H)				
Mesh	Non-uniform grids;				
	Cells across burner: Coarse, 24; Medium,				
	48; Fine, 72				
LES Model	Sub-grid kinetic energy equation				
	$C_{c} = 0.4$				
	$C_{t} = 0.05$				
Radiation Model	Finite volume method				
Soot Model	On				
Prandtl Number	0.8				
Lewis Number	1.0				
Integral Length Scale	0.42 m				
Physical Time	20 s				

Table 6.4 Summary of numerical settings for the toluene fire

6.4.2 Results and Discussions

Toluene is a heavily sooty fuel, and thus a lot of challenges are expected regarding the current combustion and soot model. Like the heptane fire, four different soot model settings, including " κ +oxid", "lam+oxid", " κ ", and "lam", would be considered, as well as two oxidation models, i.e. Eq. (3.25) and Eq. (3.26).

a. Grid Sensitivity

The centreline temperature rise and axial velocity are introduced to investigate the grid sensitivity, as displayed in Figs. 6.61 and 6.62. In Fig. 6.61, it is shown that the experimental data is in good agreement with the McCaffrey empirical model in the flame zone and the start of intermittent zone, but the discrepancy is huge in the end of intermittent zone, i.e. $z/Q^{2/5} = 0.2$. Note that this finding is consistent with the one in the previous heptane fire conducted in the same group [120], raising a doubt of the experimental credibility at that location. The predicted temperature with the "Coarse", "Medium" and "Fine" meshes generally follow the trend of McCaffrey empirical model, and the differences mainly exist in the intermittent zone and plume zone. It is observed that the predicted temperature would not vary a lot when "Medium" and "Fine" meshes are utilized, demonstrating the grid independence. Analogously, the predicted axial velocity is quite close to each other for these "Medium" and "Fine" simulations, as shown in Fig. 6.62. Note that the major difference between the predictions and McCaffrey model exists in the flame zone. As mentioned in the previous heptane fire, this could not imply the predictions are really bad, because the velocity was not measured during the experiments.



Fig. 6.61 Centerline temperature rise versus normalized height



Fig. 6.62 Normalized axial velocity versus normalized height

b. Effect of New X

Comparison of the predicted transient (at 20 s) temperature utilizing two different χ expressions is displayed in Fig. 6.63. The weak temperature rise near the fire base is also evident here, when the original expression of Eq. (2.33) is

introduced. The newly developed Eq. (2.47) is able to solve that problem, as concluded before.



Fig. 6.63 Comparison of the predicted transient (at 20 s) temperature using different expression of χ ((a) ---Eq. (2.33); (b)--- Eq. (2.47))

c. Effect of K

The transient and time-averaged κ distribution in the near field of the fire is shown in Fig. 6.64. It is also found that the averaged κ increases vertically with the increase of height. The "hump" shape is also obvious. Generally, the magnitude of the transient and average κ is predicted to be very small, say less than 0.07, demonstrating that the averaged turbulent mixing time scale is much larger than the soot chemical time scale calculated from the smoke point height, i.e. Eq. (3.18).



Fig. 6.64 The predicted transient and average κ distributions

d. Conservation of Energy

The calculated heat release rate and soot potential energy with four different soot model settings, including " κ +oxid", "lam+oxid", " κ ", and "lam", are depicted in Figs. 6.65 and 6.66, aiming to understand the effect of PaSR and soot oxidation model. Eq. (3.26) is used for the soot oxidation here. It is found that the "lam" and "lam+oxid" simulations roughly give the heat release rate of 20 kW and the soot potential energy of 104 kW, implying that the majority of energy is stored in the soot particles, not released in the domain. Given the theoretical heat release rate is set as 125 kW based on the fuel mass flow rate, one may doubt that the combustion would not be sustainable in this situation. It is explained that EDC combustion model is based on the turbulent mixing, and combustion will proceed with the presence of turbulence. In contrast, the predicted heat release rate and soot potential energy in " κ " and " κ +oxid" is around 102 kW and 22 kW. Moreover, the soot oxidation model has marginal

effect on the heat release rate and soot potential energy, particularly for the "lam+oxid" simulation compared with "lam" one.

No matter where is the energy (stored or released), theoretically the total energy should be conserved, as shown in Fig. 6.67. The total energy is estimated to be 124 kW consistent with the theoretical value based on Eq. (3.38), further demonstrating the potential of the current models.



Fig. 6.65 The predicted heat release rate with different soot model settings (Eq.

(3.26) for soot oxidation)



Fig. 6.66 The predicted soot potential energy with different soot model settings





Fig. 6.67 The predicted total energy with different soot model settings (Eq. (3.26) for soot oxidation)

e. Flame Height

The predicted flame height with four different soot model settings is illustrated in Fig. 6.68. The inclusion of PaSR and oxidation model would not have huge effects on the prediction, and the reason is because the effect of soot has been considered in the expression of flame height, i.e. Eq. (5.18). The flame height is predicted to be 1.33 m, in very good agreement with the experimental data, i.e. 1.3 m [120].



Fig. 6.68 The predicted flame height with different soot model settings (Eq.

(3.26) for soot oxidation)

f. Radiative Fraction

The predicted radiative fraction in " κ +oxid", "lam+oxid", " κ ", and "lam" simulations is displayed in Fig. 6.69. The calculated radiative fraction in "lam" and "lam+oxid" cases would be much smaller than the ones with " κ " and " κ +oxid". This must be associated with the under-prediction of heat release rate, leading to the weak temperature rise as well as the radiation emission. The impact of oxidation model is not considerable here. The radiative fraction achieved form the " κ +oxid" simulation is 0.38, in very good agreement with the experimental data, i.e. 0.35 [120].



Fig. 6.69 The predicted radiative fraction with different soot model settings (Eq. (3.26) for soot oxidation)

g. Soot Volume Fraction

The predicted transient and average soot volume fraction contour is shown in Fig. 6.70, with the application of " κ +oxid". It is clear that the transient soot volume fraction is calculated to be within a range of 0.5 ~5 ppm, and the larger values are generally located near the flame front where the temperature is thought to be higher. The non-zero values of soot volume fraction above the flame height in the average profile of Fig. 6.70 further prove that the soot particles could escape from the flame, as stated in the previous heptane fire scenario.

Comparison of the predicted mean and RMS soot volume fraction is made in Fig. 6.71 and Fig. 6.72 respectively. It is noted that Eq. (3.25) is utilized for the soot oxidation in this figure. It can be seen that the "lam" and "lam+oxid" generally over-predict the mean and RMS values 5~25 times in comparison with the measurements [120]. That is the reason why the soot potential energy is hugely over-predicted. In contrast, both the " κ " and " κ +oxid" give much better predictions as they generally have the same order of magnitude as the experiment data, except at the locations near the burner surface, say H/D=0.8. The impact of soot oxidation model is relative weak comparing with that of PaSR, particularly at the lower locations. However, it will become more evident with the increase of height, especially near the rim of the fire plume. In terms of oxidation effect, the comparison of the predicted soot volume fraction and its fluctuation with two different soot oxidation models, i.e. Eq. (3.25) and Eq. (3.26), is made in Fig. 6.73. It is noted that only " κ +oxid" soot model setting is taken into account here. At most locations both two oxidation models are capable of delivering the reasonable agreement with the experimental data. As stated before, Eq. (3.26) is recommended in this study, and its prediction may be a bit better than that using Eq. (3.25).



Fig. 6.70 The predicted transient and average soot volume fraction



Fig. 6.71 The predicted soot volume fraction at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.72 The predicted soot volume fraction fluctuation at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.73 Comparison of the predicted soot volume fraction and its fluctuation using two different oxidation models (oxid1---Eq. (3.26) for soot oxidation;

oxid2---Eq. (3.25) for soot oxidation)

h. Temperature

The mean temperature and temperature fluctuations in "lam" and "lam+oxid" simulations are predicted to be 0~500 K less than those with " κ " and " κ +oxid", as illustrated in Figs. 6.74 and 6.75. That must be associated with the under-prediction of heat release rate due to the over-estimate of soot volume fraction. It appears that " κ " and " κ +oxid" generally over-predict the mean temperature, particularly in the far field, but give very good agreement with the measurement for the temperature fluctuation. Note that the experimental data of mean temperature in the far field might be unreasonable. Taking H/D=4.3 as an example, this location is expected to be still inside the flame, provided that the

flame height is measured to be 1.3 m [120]. Therefore, the real temperature should not be very low, but it was reported to be around 500 K in the experiment. In fact, the large amount of soot particles would decrease the dependence of radiative intensities on the spectrum, leading to the decrease of experimental credibility using the spectrum-based intensities to achieve the temperature in the experimental work [120].

The predicted mean temperature and its fluctuation employing two different oxidation models, including Eq. (3.25) and Eq. (3.26), are compared in Fig. 6.76 to understand their effects. As expected, the difference between their predictions is found to be marginal. Eq. (3.26) predicts a bit lower mean temperature and its fluctuation, because less energy is generated in the domain as a result of the relatively smaller oxidation rate.



Fig. 6.74 The predicted temperature at different heights (Eq. (3.25) for soot

oxidation)



Fig. 6.75 The predicted temperature fluctuation at different heights (Eq. (3.25) for soot oxidation)



Fig. 6.76 Comparison of the predicted temperature and its fluctuation using two different oxidation models (oxid1---Eq. (3.26) for soot oxidation; oxid2---Eq.

(3.25) for soot oxidation)

6.5 METHANE FIRES

6.5.1 Problem Descriptions

A series of methane fires with the diameter of 30 cm, conducted by McCaffrey [117] and Cox [122], are considered here. In total, there are 6 cases included in this section, with the fire power of 18.0 kW, 21.7 kW, 33.0 kW, 44.9 kW, 47.0 kW, and 57.5 kW. A cylindrical computational domain of 1.8 m in diameter and 3.6 m in height was used to minimize the influence of open boundaries, as displayed in Fig. 6.77. Non-uniform meshes were employed similarly like the one in Fig. 6.2. Note that the temperature boundary condition for the gas methane inlet was set as fixed enthalpy flux rather than fixed temperature, aiming to mimic temperature build-up over the inlet. Two types of boundary conditions shown in Fig. 6.77 were used in the calculations: free boundary conditions on the surface of the open domain and prescribed mass flow rate profiles at the fuel exit surface. The laminar smoke point height is set as 0.29 m for the fuel methane, as explained before. Both turbulent Prandtl number and Schmidt number were set as 0.8. The soot model was switched on with PaSR adopted for the soot formation and with Eq. (3.26) for the soot oxidation, as recommended before. Optically thin assumption [105] was activated, as the methane flame is not sooty. The physical time was chosen to be 20 s to ensure the flame is fully developed. All the above settings are summarized in Table 6.5.



Fig. 6.77 Schematic of the domain for the methane fires

Table 6.5 Summary of numerical settings for the methane fires

Experimentalist	McCaffrey and Cox							
Fuel	Methane							
Smoke Point Height	0.29 m							
Fire Size	30 cm							
Theoretical HRR (kW)	18.0	21.7	33.0	44.9	47.0	57.5		
Integral Length Scale (m)	0.19	0.21	0.25	0.28	0.28	0.31		
Inlet Temperature	Fixed enthalpy flux							
Computational Domain	1.8 m (D) × 3.6 m (H)							
Mesh	Non-uniform grids;							
	Cells across burner: Coarse, 15; Medium, 30; Fine 45							
W	Sub-grid kinetic energy equation							
LES Model	$C_c = 0.4$							
	$C_{k} = 0.05$							
Radiation Model	Optically thin assumption							
Soot Model	On							
Prandtl Number	0.8							
Lewis Number	1.0							
Physical Time	20 s							

6.5.2 Results and Discussions

a. Grid Sensitivity

In terms of grid sensitivity, a 44.9 kW methane fire is arbitrarily chosen here. Three different meshes were applied to the domain, denoted as "Fine", "Medium", and "Coarse", and the number of cells across the burner was selected to be 45, 30 and 15 accordingly. Centreline temperature rise and axial velocity with the variation of grid size is plotted in Figs. 6.78 and 6.79. The "Coarse" prediction generally follows the trend of experimental data and the empirical model, but its value is a bit larger. This may be relevant to the over-prediction of total dissipation rate, causing the sharp increase of mass transfer rate, i.e. Eq.
(2.22), for the combustion model. One could observe that the predicted temperature gets very close when "Medium" and "Fine" meshes are applied, and so does the predicted axial velocity. That means the independence of the grid. Note that the fluctuating behaviour of the curves regarding the "Coarse" mesh should be linked to the interpolation during the data extraction, and it wouldn't influence the grid analysis.



Fig. 6.78 Centerline temperature rise versus the normalized height



Fig. 6.79 Normalized axial velocity versus normalized height

b. Effect of New x

The new χ expression is also tested here. Comparison of the predicted transient (at 20 s) and average temperature applying the new and original χ expressions is presented in Fig. 6.80. One could clearly see the lifted flame from the fuel burner once the original formula is adopted, and this finding is more evident than that of heptane and toluene fires. This should be linked to the smaller molar weight of fuel methane, inducing the lower gas density. It is proved again that the new expression is capable of anchoring the flame to the burner, and making the average temperature distribution more plausible.



Fig. 6.80 Comparison of the predicted transient and average temperature (at 20 s) using different expression of χ ((a),(b) ---Eq. (2.33); (c),(d)--- Eq. (2.47))

c. Soot Effect

Methane is a very special fuel, of which the smoke point height is hardly captured. The value of 29 cm in Table. 3.1 is estimated according to the radiative fraction comparison between methane and ethane [32], not from the direct measurement. In the similar study, Yao [84] concluded that the original soot formation coefficient calculated from the smoke point height, i.e. $A_t/L_{sp} = 1.5E - 5$,

would over-predict the soot volume fraction by one order of magnitude in the turbulent methane jet flames, and presented a value of 1E-6 for that soot formation coefficient. It is worth mentioning that his conclusion was based on the jet flame calibration, which is momentum controlled, and it might thus be inappropriate in the buoyancy-driven fire scenarios.

Those two values are tested in this 44.9 kW methane fire, and the corresponding predicted transient and average soot volume fraction is illustrated in Fig. 6.81. It is summarized that the peak average soot volume fraction is calculated to be around 0.04 ppm, if the coefficient of 1E-6 calibrated by Yao [84] is used. In contrast, the relevant prediction would be around 0.5 ppm for the coefficient calculated from the smoke point height. Plenty of previous studies [81, 123-125] suggest that the soot volume fraction for the small/medium methane fire ranges from 0.1 ppm to 1 ppm. Hence, the coefficient calibrated from the jet flame is not applicable to this buoyancy controlled fire. The value achieved from the smoke point height is employed in all the small/medium methane fires.



Fig. 6.81 The predicted transient and average soot volume fraction (PPM) using two different soot model settings ((a) and (b) --- $A_f/L_{sp} = 1.0E - 6$; (c) and (d) ---

$$A_f / L_{sp} = 1.5E - 5$$
)

d. Radiative Fraction

As a matter of fact, the methane fire is relatively clean, and the optically thin assumption for the radiation model is thus understandable. Theoretically, the spectrum band dependence of the radiative intensity should be considered for this kind of flame, but this process is very time consuming. The concept of optically thin assumption is to disregard the calculation of the incident radiation from a series of radiative intensities, and further to neglect the radiation absorption. Therefore, only radiation emission effect is accounted for in this circumstance.

Here three different methods to enclose the radiation source term in the energy equation are included, denoted as "Thin-soot", "Thin-noSoot", and "RTEsoot". "Thin-soot" means the application of optically thin assumption, as well as the activation of soot model. Based on this "Thin-soot" method, "Thin-noSoot" implies the deactivation of soot model, while "RTE-soot" represents the calculation of RTE. It is worth reminding that the fire mixture is assumed to be grey for the absorption coefficient calculation in "RTE-soot". Comparison of the predicted radiative fraction using these three methods is shown in Fig. 6.82. The average radiative fraction is calculated to be 0.31 in "Thin-soot", and this value would decrease to 0.258 for the case without the presence of soot particles, i.e."Thin-noSoot", proving that the gas phase radiation is dominant in this methane fire scenario. In contrast, "RTE-soot" gives the value of 0.26, reflecting the participation of absorption in the radiation source term is relatively weak, by comparing with the emission. Additionally, oscillations of the "RTE-soot" transient curve are believed to be due to the solving frequency of 10, which don't influence our analysis.



Fig. 6.82 The predicted radiative fraction with the optically thin assumption or the calculation of RTE

e. Flame Height

The calculated flame height with or without soot model is summarized in Fig. 6.83, and all the 6 fire powers described before are included. Here these flame height calculations are compared with the McCaffrey empirical model expressed below, as there is no experimental data:

$$L_f = 0.235Q^{2/5} - 1.02D \tag{6.8}$$

It is found that the predictions agree very well with the linear relationship between L_{f} and $Q^{2/5}$. Furthermore, the predictions are a bit smaller than the corresponding values using the empirical model. One may also conclude that the presence of soot particles would lead to the reduction of flame height, as a consequence of combustion incompleteness.



Fig. 6.83 Comparison of the predicted flame height with Heskestad model (Prediction-1: soot model; Prediction-2: no soot model)

f. Centreline Temperature and Velocity

The predicted centreline mean temperature rise and temperature fluctuation, compared with the experimental data and McCaffrey empirical model as a function of the normalized height, are demonstrated in Fig. 6.84 and Fig. 6.85, respectively. Overall, the calculated mean temperature is in very good agreement with the experimental data, as well as the derived McCaffrey model. Note that the minor difference between the predictions and empirical model is mainly existent in the flame zone. In terms of temperature fluctuation, we only have the experimental data for 18.0 kW and 47.0 kW cases, conducted by Cox [122]. According to these data available, it is found that the temperature fluctuation is over-predicted in the flame zone, and agrees well with the measurement in the intermittent and plume zones. Moreover, the comparison of the predicted axial velocity along the centreline with the experimental data further demonstrates the capability of the current models, as the good agreement is observed in Fig. 6.86.



Fig. 6.84 Centerline temperature rise versus normalized height



Fig. 6.85 Temperature fluctuation versus normalized height



Fig. 6.86 Normalized axial velocity versus normalized height

g. Radial Temperature and Velocity

The radial temperature and velocity distributions at different elevations are covered in Figs. 6.87 and 6.88. Note that there is only limited experiment data for 18.0 kW and 47.0 kW cases. Overall, the good agreement is also obtained. However, it appears that the velocity is a bit under-predicted, especially at the higher location, say H=0.8 m. The predicted plume width may be smaller than the measurement, based on these insufficient experimental data.



Fig. 6.87 Comparison of the predicted temperature and vertical velocity with the measurements for a 18.0 kW fire



Fig. 6.88 Comparison of the predicted temperature and vertical velocity with the measurements for a 47.0 kW fire

6.6 ENCLOSED METHANE FIRE

6.6.1 **Problem Descriptions**

The 1 m diameter methane fire scenario tested by Tieszen [126] is chosen in this section. The experiments were performed in a large building at Sandia Laboratory in the USA, which is nominally a 6.1 m cube with a one-metre diameter burner located near the centre of the facility, 2.45 m above the floor. The facility and burner layout have been designed to approximate an unconfined fire on an infinite ground plane even though the burner was in an enclosure. The vertically oriented airflow comes from 16 segments in the annular ring 1.75 m below the burner surface. At the surface of the annular ring, the vertically oriented airflow was 0.30 m/s. This was expected to decelerate as its area broadens nearer to the burner surface. Strictly speaking, the test case cannot be considered as an unconfined fire although it is well ventilated. The circular bund surrounding the burner may act to limit the radial expansion of the fire plume and then stretch the fire in the vertical direction. The elevated position of the burner and the vertical air supply from the bottom would also lead to air ingress into the fire region not only from the outer region but also from lower surroundings. These geometrical details were generally neglected in the previous LES simulations of this particular case [127-129]. In this study, the possible effect of deviation from the experimental setup will be discussed.

A cylindrical computational domain was adopted with 2 m in diameter, and 4.5 m in height, quite analogous to Fig. 6.36. Note that the width of domain was set as same as the one by Xin et al. [127]. The structure of meshes was similar to that in Fig. 6.2. Three different meshes were applied to the domain,

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denoted as "Fine", "Medium", and "Coarse", and the number of cells across the burner was selected to be 72, 36 and 18 accordingly. An inlet mass flow rate is set as 0.0519 kg/s, and the theoretical heat release rate is thus calculated to be 2.59 MW if the combustion is assumed to be complete. The bottom plane except the burner inlet is set as solid wall and all the other planes are defined as pressure/outlet boundaries, as shown in Fig. 6.36. The ambient air assumed to be in quiescent condition is set at 277K and 81.1 kPa. The inlet temperature boundary is set as same as that in the previous methane scenarios. The laminar smoke point height is set as 0.29 m for fuel methane, as demonstrated before. Both turbulent Prandtl number and Schmidt number were set as 0.8. The soot model was activated with the application of PaSR to the soot formation, and of Eq. (3.26) to the soot oxidation. Optically thin assumption [105] was also activated. The physical time was set as 30 s. All the above settings are summarized in Table 6.6.

Experimentalist	Tieszen
Fuel	Methane
Smoke Point Height	0.29 m
Fire Size	1 m
Mass Flow Rate	0.0519 kg/s
Theoretical HRR	2.59 MW
Inlet Temperature	Fixed enthalpy flux
Computational Domain	2 m (D) × 4.5 m (H)
Mesh	Non-uniform grids; Cells across burner: Coarse, 18; Medium, 36; Fine, 72
LES Model	Sub-grid kinetic energy equation $C_e = 0.4$ $C_k = 0.05$
Radiation Model	Optically thin assumption

Table 6.6 Summary of numerical settings for the enclosed methane fire

Soot Model	On	
Prandtl Number	0.8	
Lewis Number	1.0	
Integral Length Scale	1.4 m	
Physical Time	30 s	

6.6.2 Results and Discussions

a. Grid Sensitivity

Comparison of centreline temperature rise and axial velocity using different grid size is presented in Figs. 6.89 and 6.90. As concluded before, the "Coarse" mesh tends to over-predict the temperature and axial velocity. Grid independence is observed, as the "Medium" and "Fine" curves get converged for both the predicted temperature and velocity. The fuel rich core induced weak temperature rise in the flame zone is evident here. It is also illustrated that the McCaffrey empiric model over-estimates the axial velocity in the flame zone, while the predictions agree very well with the experimental data.



Fig. 6.89 Centerline temperature rise versus normalized height



Fig. 6.90 Normalized axial velocity versus normalized height

b. Effect of New χ

The effect of χ expression is also examined here. Comparison of the predicted transient (at 30 s) temperature utilizing the new and original χ expressions is displayed in Fig. 6.91. The flame lifted from the fuel burner is clearly found. As clarified before, the relatively small molar weight of fuel methane result into this obvious lifted phenomenon. In sharp contrast, the new expression is proved once again to be capable of tackling this problem.



Fig. 6.91 The predicted transient (at 30 s) temperature using the different expression of χ ((a)---Eq. (2.33); (b)--- Eq. (2.47))

c. Geometric Effect

During the test, the vertically oriented airflow of 0.3 m/s was applied at the surface of the annular ring consisted of 16 segments, which are located 1.75 m below the burner surface. So far, we still don't know whether this experimental setting would have some effect or not. Generally, the vertical airflow was neglected in the previous LES simulations of this particular case [127-129]. In this work, we set up two cases to check this geometric effect. Bear in mind that "Total" means the simulation results considering the vertical velocity and the entire experimental geometry, while "Part" represents results of the simplified geometry, which is set up by the previous investigators [127-129]. Note that the number of meshes in the "Part" domain is kept the same as that of "Total" in the corresponding region. It is shown in Fig. 6.92 that in both cases the predicted vertical velocity and horizontal velocity agree very well with the measurements. The presence of the vertical airflow on the ground has a minor stretching effect rather than a pushing effect on the fire plume, as found in the vertical velocity profiles. The relatively long distance between the burner and the ground inlet may significantly reduce the vertical velocity at the elevation of burner, and hence the fire plume width near the burner could expand a little bit in order to get more oxygen to sustain the combustion. This point is further verified by the fact that the horizontal velocity in "Total" simulation is predicted to be a bit larger than that in "Part" simulation. Overall, however, the velocity difference due to the treatment of the experimental geometry is found to be marginal.



Fig. 6.92 Comparison of the predicted velocity using different geometry

d. Puffing Phenomenon

The vertical velocity is monitored during the simulation, and then compared with the corresponding measurement, as shown in Fig. 6.93. The periodic puffing behaviour is clearly found in the prediction, and the periods of puffing cycles vary somewhat from cycle to cycle, as addressed in the relevant experimental work [126]. The average period is predicted to be 0.65 s, as 11 cycles exist within 7.2 s. This value is a bit larger than the measurement of 0.62 s [126], but a little smaller than the estimated value of 0.67 s from Pagni's empirical model [118]. Additionally, the magnitude of vertical velocity is in good agreement with the experimental data at most time points. The predicted and measured four phases of a puffing cycle are demonstrated in Fig. 6.94. Note that the start of this cycle is arbitrarily chosen. It is found that the movement of large vortices, which is a dominant factor in buoyancy-driven fires, in the prediction is consistent with the measurement, and the evolution of the puffing behaviour is thus well captured.



Fig. 6.93 Vertical velocity history at the height of 50.5 cm (Row 1: experiment;

Row 2: prediction)



Fig. 6.94 Comparison of the velocity vector field (Column 1---experiment;

Column 2---prediction)

e. Velocity

Comparison of the predicted vertical and horizontal velocity with the measurement is made in Fig. 6.95. It appears that the prediction is symmetric about the burner centreline, and the iso-value curves in the measurement are generally not as smooth as the ones in the prediction. The reason might be due to flow perturbations in the surroundings. Overall, the predictions are in reasonable agreement with the experimental data. However, the simulated and measured vertical velocity profiles demonstrate that the predicted flame width is around 10 cm wider than the measurement. Both the vertical and horizontal velocity are slightly over-predicted, by comparing the relevant iso-value curves.



Fig. 6.95 Comparison of the predicted vertical and horizontal velocity with the measurement ((a),(b)---vertical velocity, m/s; (c),(d)---horizontal velocity, m/s;

Column 1---prediction; Column 2---experiment)

f. Turbulent Properties

Figure 6.96 describes the comparison of the predicted and measured turbulent stresses, including $\overline{u'_z u'_z}$, $\overline{u'_y u'_y}$, and $\overline{u'_y u'_z}$, which are important factors to evaluate the capability of the current models, in particular LES model. Both the prediction and measurement show that turbulent stress $\overline{u'_z u'_z}$ increases away from the burner surface within the plotted region, and that two off-axis peaks at the same vertical distance are present. However, its magnitude is generally over-

predicted, particularly in the centreline area starting from 30 cm above the burner, implying that the fire fluctuates along the vertical direction more strongly in the prediction than that in the measurement. Additionally, the wider flame width in the prediction is also evident here.

On the contrary, the turbulent stress $\overline{u'_y u'_y}$ is a bit under-predicted, and two off-axis peaks expand a bit consistent with the wider predicted flame width. Regarding the stress $\overline{u'_y u'_z}$, the main discrepancy exists near the fire base. The prediction presents two groups of clustered iso-lines distributed symmetrically, and the reason should be associated with the buoyancy induced air entrainment. However, this phenomenon is not shown in the relevant measurement profile, and it might be due to the relatively small magnitude. The turbulent kinetic energy is a bit over-predicted, especially near the centerline area, as illustrated in Fig. 6.97.



Fig. 6.96 Comparison of the predicted turbulent stress with the measurement ((a),(b)--- $\overline{u'_{2}u'_{z}}$, m²/s²; (c),(d)--- $\overline{u'_{y}u'_{y}}$, m²/s²; (e),(f)--- $\overline{u'_{y}u'_{z}}$, m²/s²; Column 1--prediction; Column 2---experiment)



Fig. 6.97 Comparison of the predicted total turbulent kinetic energy k_{total} with the measurement ((a)---experiment; (b)---prediction)

Chapter 7

Large Scale LNG Pool Fires

7.1 INTRODUCTION

With the growing importance of LNG in the world energy arena, additional research is necessary to quantify the hazards associated with a potential spill either on land or water so industry can make informed decisions about the siting of LNG terminals and protecting existing terminals and tankers. In an expert panel convened in US to rank the need for research on LNG and suggest future research priorities to determine the public safety impact of an LNG spill, large fire phenomena was ranked as having the highest priority.

Previous studies on LNG fires have primarily been based on experimental tests and semi-empirical models [108, 130-139]. While numerical simulations based on field modeling techniques are now routinely used for the simulations of many other fire scenarios, limited attempts have been reported on LNG or large scale pool fires. The major barrier is the relatively large size of the domain, the lack of robust combustion and soot models and complex radiation characteristics of LNG fires. The inter-connection of soot and radiation in such large fires also demands close coupling of the two in any rigorous modeling approach.

For the calculation of thermal radiation hazards distances around large scale LNG pool fires, semi-empirical models such as the solid flame model (SFM) are widely used. SFM assumes the fire as a circular cylinder (vertical or

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tilted) of diameter equal to the fire size and of axial length representing the visible plume of the fire. Although semi-empirical approaches can estimate the radiation hazards, they cannot predict the reduction of radiation due to smoke obscuration, and also fail to properly account for the dynamics of large LNG fires. Moreover, as commented by Raj [138] it is erroneous to extrapolate results especially thermal radiation emissions from small scale experiments for predicting the characteristics of large size fires. CFD approach should provide a good alternative for such large LNG fires.

In this chapter, we will apply the combustion and soot model, which are validated in the small/medium scale fire scenarios, to a series of large scale LNG pool fires with the pool diameters of 14 m, 21 m, 35 m and 56 m. The soot model will be activated with PaSR adopted for the soot formation and with Eq. (3.26) for the soot oxidation. The FVM, rather than the optically thin assumption, will be used to predict radiative heat flux.

7.2 CHINA LAKE 14 m POOL FIRE

7.2.1 Problem Descriptions

Numerical simulations are based on Test 12 in the China Lake test series which involved spilling LNG on water in a 50 m \times 50 m \times 1 m pond. The test was the only one in the series conducted in no-wind condition and the only test for which both the wide angle radiometer (WAR) data and narrow angle radiometer (NAR) data were analyzed to obtain surface emissive power (SEP). The volume of LNG spilled was 5.7 m³ with the rate of 0.07 m³/s. The fire base diameter is 14 m and the visible flame length was measured as 44.0±6.3 m. The average LNG burning rate was measured as 4.94E-4 m/s, corresponding to the mass loss rate per area of 0.22 kg/m^2 s. The WAR was directed at 1.5 m above the fire base and 30 m from the fire centre while two NAR were also set at the location 30 m far from the pool centre but with height of 4.6 m and 6.2 m above the fire base.

According to the dimension of the LNG pool fire in the China Lake Tests, a cylindrical domain, with diameter of 80 m and height of 200 m, was employed. A circular pool with diameter of 14 m was located in the middle of the floor. The number of cells was set as 26, 52 and 78 on the burner for the "Coarse", "Medium" and "Fine" cases, respectively. The boundaries of the domain except the ground floor were defined as 'opening', equivalent to Fig. 6.36, which means that fire smoke and fresh air could exchange across the boundary. Since the China Lake Tests were conducted on water, the inlet temperature is set as the boiling temperature of water, i.e. 373 K. The turbulent Prandtl number and Schmidt number were set as 0.8, as same as the previous methane fire scenarios. The simulations were found to reach quasi-steady state after 15 s and but were continued for another 35 s to allow the fire to be fully developed. All the above settings are summarized in Table 7.1.

China Lake	
Methane	
0.29 m	
14 m	
0.22 kg/m ² s	
2.59 MW	
373 K	
80 m (D) × 200 m (H)	
Non-uniform grids;	
	China Lake Methane 0.29 m 14 m 0.22 kg/m²s 2.59 MW 373 K 80 m (D) × 200 m (H) Non-uniform grids;

Table 7.1 Summary of numerical settings for the China Lake 14 m LNG fire

	Cells across burner: Coarse, 26; Medium, 52; Fine, 78
LES Model	Sub-grid kinetic energy equation $C_{e} = 0.4$ $C_{k} = 0.05$
Radiation Model	Finite volume method
Soot Model	On
Prandtl Number	0.8
Lewis Number	1.0
Integral Length Scale	18.83 m
Physical Time	50 s

7.2.2 Results and Discussions

a. Grid Sensitivity

The centreline temperature rise and axial velocity are introduced to understand the grid sensitivity, as depicted in Figs. 7.1 and 7.2. It is also found that the "Coarse" mesh slightly over-estimates both the temperature and axial velocity, as observed in the last chapter. This should also be associated with the over-prediction of SGS kinetic energy. The predicted temperature would not change hugely when "Medium" and "Fine" meshes are utilized, implying the grid independence. It is noted that the predicted temperature with the "Coarse", "Medium" and "Fine" meshes generally follow the trend of McCaffrey empirical model, particularly in the plume zone, while there is considerable difference existent in the flame zone and intermittent zone. Due to the presence of fuel rich core in the flame zone, the temperature rise would be relatively slow with the increase of height, and it is thus not possible to maintain the same value like in the McCaffrey empirical model. Similarly, it is seen that the predicted axial velocity curves are almost the same for the "Medium" and "Fine" simulations. Moreover, the predicted flame height with the variation of grid size is also examined here, as illustrated in Fig. 7.3. It is found that the grid size may have some effect on the amplitude of the flame height fluctuation, but would not hugely change the average value. Therefore, the "Medium" and "Fine" meshes are believed to be adequate. The average flame height is predicted to be around 50 m, consistent with the corresponding measurement, i.e. 44.0 ± 6.3 m.



Fig. 7.1 Centerline temperature rise versus normalized height



Fig. 7.2 Normalized axial velocity versus normalized height



Fig. 7.3 The predicted flame height with different grid size

b. Soot Formation Coefficient

Technically, the soot formation coefficient A_f/L_{sp} in Eq. (3.17) should be calculated from the smoke point height L_{sp} of a specific fuel. Although the soot formation coefficient based on the smoke point height of 29 cm, i.e.

 $A_f/L_{sp} = 1.5E - 5$, performs well in the small/medium scale methane fire scenarios, its capability in the large scale fires needs to be further investigated. The predicted soot yield using the coefficient $A_f/L_p = 1.5E - 5$ is shown in Fig. 7.4. It is found that the value generally varies from 0.2 to 0.4, leading to the average value of 0.3. This prediction is thought to be approximately 2.5 times bigger than the corresponding estimation by Raj [138], i.e. 0.12. Therefore, the coefficient calculated from the smoke point height is prone to over-predict the soot production, raising the challenge of applying the soot model developed and validated in small/medium fires to the large scale fires. In this work, that coefficient is tuned to be 3.0E-6, as one can find the predicted average soot yield is roughly 0.12, equal to the estimated value by Raj [138]. The effect of that tuned coefficient on the soot volume fraction and temperature is inspected in Figs. 7.5 and 7.6. It is evident that both the transient and average soot volume fraction are decreased by nearly 4 times. The predicted average value with the coefficient of 3.0E-6 has the order of magnitude of 0.1 ppm, which is also close to the relevant forecast of 0.18 ppm by Raj [138]. Therefore, the tuned coefficient of 3.0E-6 is recommended for large scale LNG fires, and will be utilized throughout this chapter.

The predicted flame zone, which may be identified from the critical flame temperature of 1000 K, is a bit larger, as demonstrated in Fig. 7.6. The reason must be associated with the decrease of soot potential energy due to the reduction of soot volume fraction, causing the increase of heat release rate based on the law of conversation of energy.



Fig. 7.4 The predicted soot yield with different soot formation coefficient



Fig. 7.5 The predicted transient and average soot volume fraction with different soot formation coefficient (Row 1: $A_f/L_{sp} = 1.5E - 5$; Row 2: $A_f/L_{sp} = 3E - 6$)



Fig. 7.6 The predicted average temperature with different soot formation coefficient ((a): $A_f/L_{sp} = 1.5E - 5$; (b): $A_f/L_{sp} = 3E - 6$)

c. Conservation of Energy

The curves of heat release rate, soot potential energy and total energy against time are plotted in Fig. 7.7. It is observed that around 214 MW of energy is stored in the soot particles, and the released energy, due to the gas phase combustion and soot oxidation, is estimated to be 1508 MW. Thus the total energy would be 1722 MW. This is in very good agreement with the theoretical value calculated from the inlet mass flow rate, i.e. 1715 MW.



Fig. 7.7 The predicted energy curves versus time

d. Puffing Cycle

The axial velocity is monitored during the simulation, and its time history is demonstrated in Fig. 7.8. The periodic puffing behaviour is evident here, and the periods of puffing cycles vary from cycle to cycle, similarly like the finding in the 1 m methane fire. The average period is estimated to be 2.3 s, as roughly 11 cycles are found within 25 s. Note that one could also observe the existence of these 11 cycles from Fig. 7.7. This predicted value is very close to the estimation according to Pagni's empirical model [118], i.e. 2.5 s. The predicted vector field within 2.5 s is illustrated in Fig. 7.9, and the start of this period is arbitrarily chosen. The large vortices initiated from the burner rim are clearly found, of which the formation, rise and break-up actually determine the puffing behaviour of a buoyancy-driven fire.


Fig. 7.8 The predicted axial velocity at the height of 20 m above the ground



Fig. 7.9 The predicted velocity vector field within 2.5 s

e. Surface Emissive Power

It is known that three methods, including "Flame Emissivity", "Surface Heat Flux" and "Surface Emissivity", are developed in this study to achieve the surface emissive power, which is an extremely important quantity in the LNG pool fires. As a matter of fact, in these large scale fires the direct measurement of common quantities, such as temperature, velocity and soot volume fraction, becomes impossible, let alone the turbulent ones. Therefore, the SEP data from the WAR or NAR, implicitly representing the radiative character which indirectly links to the combustion and soot production, is very valuable in this regard. Moreover, this quantity is widely used in the empirical model to roughly estimate the radiative heat flux at some location.

The predicted surface emissive power with three different methods is depicted in Fig. 7.10. It is found that the "Surface Emissivity" method delivers relatively low magnitude of SEP. Bear in mind that this method is based on the local emissivity, which is calculated from the local absorption coefficient and local beam length. Actually, the grid size is assumed to be equal to the local beam length, and the predicted value would thus change significantly with the variation of grid size. Technically, the smaller grid size would give rise to the lower local emissivity due to the smaller beam length as derived from Eq. (4.33), and the predicted SEP would be lower provided that the grid size is already sufficient enough to ensure the flame temperature would not vary hugely. From this point of view, this method is not recommended for the SEP calculation.

It is found that the prediction using "Flame Emissivity" and "Surface Heat Flux" is very close to each other, with the average value of 275 kW/m^2 and 269 kW/m², respectively, both of which are in reasonable agreement with the measured value, i.e. $220\pm47 \text{ kW/m}^2$. The "Flame Emissivity" method only relies on the predicted flame temperature, as the total flame emissivity is predicted to be 1 at all times. In this simulation, the average beam length and absorption coefficient is estimated to be 11.9 m and 3.2 m⁻¹. The corresponding flame emissivity of 1 can be achieved from Eq. (4.24). It is worth mentioning that Drysdale [109] made similar conclusion about this emissivity in large scale fires. Theoretically, the "Surface Heat Flux" method is an ideal one to calculate SEP, but a lot of challenges need to be confronted regarding the identification of outer flame surface. The potential block effect due to the existence of soot particles

would make this method more difficult. The coefficient C_{sr} is tuned to be 0.15 in this large scale scenario, and it would be default value for the rest of the cases in this Chapter.



Fig. 7.10 The predicted surface emissive power using three different methods

7.3 PHOENIX 21 m POOL FIRE

7.3.1 Problem Descriptions

In this test [136], 58.0 m³ LNG was discharged on water through a 15 inch pipe. The flow rate initially was about 0.061 m³/s and increased throughout the test, reaching 0.123 m³/s at the end of the test. During the steady-state fire interval, the average flow rate from the reservoir was 0.119 m³/s, yielding an average mass discharge rate of 50.0 kg/s from the reservoir. The liquid mass flow rate from the diffuser was slightly less at 48.4 kg/s due to two phase flow and the generation of methane vapor. The steady-state pool area yielded an equivalent circular diameter of 21.4 m, and the regression rate was 0.14 kg/m²s. Note that this mass loss rate was approximately 66 % of the value used for the reservoir

design criteria (0.212 kg/m²s). During the test, the average wind speed was 4.8 m/s, tilting the flame plume to some direction. The average length was measured as 60~70 m, yielding an L/D ratio of 2.8~3.3. The average height and tilt angle was around 34 m and 50°, respectively. Narrow view radiometers corrected for transmission losses measured a spot-average SEP of 228 kW/m². A flame-averaged SEP was determined by correlating view factor information from video analysis with the wide-angle radiometer data, yielding an average overall SEP of 270 kW/m².

A cylindrical computational domain with the size of 200 m in diameter, 100 m in height was set to ensure that the influence of outflow boundaries is negligible as displayed in Fig. 7.11. Non-uniform meshes were employed with grid points clustered around the burner centre and their size gradually increased in the radial and vertical direction, similarly like Fig. 6.2. The number of grid points across the burner was set as 36, 54 and 72 for "Coarse", "Medium" and "Fine" simulations, respectively. In the "Fine" case, 264 cells were applied through the diameter of whole domain, while 120 cells were introduced along the height direction. The atmospheric velocity profile, i.e. Eq. (5.20), was applied to the cross wind inlet boundary as shown in Fig. 7.11, with H_r and $u_{in}(H_r)$ equal to 9.0 m and 4.8 m/s, respectively. Meanwhile, the initial velocity field inside the domain was set as the same to improve numerical stability. The inlet mass flow rate is set as 50.355 kg/s according to the test, giving the theoretical heat release rate of 2518 MW. The integral length scale is calculated to be 22.02 m based on Eq. (2.28). The inlet temperature is set as the boiling temperature of water, i.e. 373 K. Both turbulent Prandtl number and Schmidt number were set as 0.8. The physical time was set as 50 s to ensure the fire is fully developed, while the averaging process starts from 25 s after ignition. All the above settings are summarized in Table 7.2.



Fig. 7.11 Schematic of the domain for the Phoenix 21 m LNG fire

Location	Phoenix	
Fuel	Methane	
Smoke Point Height	0.29 m	
Fire Size	21 m	
Mass Flow Rate	50.355 kg/s	
Theoretical HRR	2518 MW	
Computational Domain	200 m (D) × 100 m (H)	
Mesh	Non-uniform grids; Cells across burner: Coarse, 36; Mediu 54; Fine, 72	
Fuel Inlet Temperature	373 K	
Wind Inlet Velocity	Atmospheric velocity profile	
LES Model	Sub-grid kinetic energy equation $C_{\varepsilon} = 0.4$ $C_{k} = 0.05$	
Radiation Model	Finite volume method	
Soot Model	On	
Prandtl Number	0.8	

Lewis Number	1.0
Integral Length Scale	22.02 m
Physical Time	50 s

7.3.2 Results and Discussions

a. Grid Sensitivity

In case of cross wind, the flame would tilt to some direction, and the centreline temperature rise and axial velocity cannot be applied for the grid sensitivity study. The calculated flame height with the variation of grid size is depicted in Fig. 7.12. It is found that the decrease of grid size would increase the fluctuation of the flame height, but would not have a huge effect on the timeaveraged value, which is around 27.4 m. This value is slightly lower than the measurement of 34 m. Moreover, the variation of grid size has very weak effect on the predicted flame tilted angle from the vertical direction, as shown in Fig. 7.13. The time-averaged angle is calculated to be 57.8°, slightly greater than the measurement, i.e. 50°, and hence the cross wind have a bit more impacts on the flame behaviour during the simulation than that in the experiment. Combing with the flame angle and flame height, one could work out the averaged flame length, which is expressed as 27.4 m/cos57.8°, i.e. 51.4 m. This value is still a bit lower than the measurement of 60~70 m. As explained in Chapter 5, the pressure term is neglected in the energy equation for the cross wind scenarios, and the effect of compressibility cannot thus be accounted for. Ideally, specific outlet boundary conditions for the pressure and velocity need to be developed in these scenarios, if the fully compressible solver is considered. Unfortunately, we are still not fully aware of the effect of disregarding the pressure term on the energy transport, as it could be examined only if one has very sophisticated pressure and velocity boundary conditions.



Fig. 7.12 The predicted flame height with different grid size



Fig. 7.13 The predicted flame angle with different grid size

b. Soot Formation Coefficient

The impact of soot formation coefficient A_t/L_m is also investigated here. The predicted soot yield with two coefficients presented above is shown in Fig. 7.14. It is found that the transient value generally ranges from 0.3 to 0.4, if the coefficient, i.e. 1.5E-5, calculated from smoke point height is adopted. This prediction is believed to be roughly 2.3~3.1 times bigger than the preliminary estimation by Raj [138], i.e. 0.13. Note that that estimation is based on the 20 m LNG pool fire on land, while the scenario we considered here is a fire with the same size on water. Nevertheless, it should be acceptable that the coefficient tends to over-estimate the soot production, as concluded before. In contrast, the coefficient of 3.0E-6, tuned from the last LNG scenario, could produce the average soot yield of 0.11, in reasonable agreement with that Raj's estimation. The influence of that tuned coefficient on the soot volume fraction and temperature is examined in Figs. 7.15 and 7.16. It is still clear that both the transient and average soot volume fraction are decreased by nearly 4 times. The predicted average value with the coefficient of 3.0E-6 has the order of magnitude of 0.1 ppm, which agrees well with Raj's empirical estimation of 0.19 ppm [138].

With a setting of critical flame temperature of 1000 K, the predicted flame zone would become larger due to that decrease of soot formation coefficient, as illustrated in Fig. 7.6. This is because more energy is artificially released from the soot potential energy, as explained before. One could also observe that the "iso-value" curves tend to approach the vertical direction for the prediction with the coefficient of 3.0E-6, implying the flame angle becomes smaller. It is known that the more released energy would correspond to the higher temperature, causing lower density if the static pressure is kept the same. The induced bigger density difference would give rise to the stronger buoyancy exerted along the vertical direction, and thus pull the flame closer to the vertical.



Fig. 7.14 The predicted soot yield with different soot formation coefficient





Fig. 7.15 The predicted transient and average soot volume fraction with different soot formation coefficient (Row 1: $A_f/L_{sp} = 1.5E - 5$; Row 2: $A_f/L_{sp} = 3E - 6$; dashdot line: burner rim)



Fig. 7.16 The predicted average temperature with different soot formation coefficient ((a): $A_f/L_{sp} = 1.5E - 5$; (b): $A_f/L_{sp} = 3E - 6$; dash-dot line: burner rim)

c. Conservation of Energy

The predicted heat release rate, soot potential energy and total energy against time are demonstrated in Fig. 7.17. Note that the coefficient of 3.0E-6 is applied. It is shown that around 280 MW of energy is stored into soot particles, and the released energy from gas phase combustion and soot oxidation is estimated to be 2205 MW. Thus the total energy would be 2485 MW, which agrees reasonably with the theoretical value calculated from the inlet mass flow rate, i.e. 2518 MW.



Fig. 7.17 The predicted energy curves versus time

d. Surface Emissive Power

The predicted surface emissive power utilizing three different methods is depicted in Fig. 7.18. The "Flame Emissivity" method predicts the average SEP of 255 kW/m², in reasonable agreement with the experimental data, i.e. 270 kW/m². As found before, the "Surface Emissivity" method gives relatively low magnitude of SEP, with the average value of 177 kW/m². The prediction with "Surface Heat Flux" is somewhere in-between, i.e. 214 kW/m². Therefore, it is proved again that the "Flame Emissivity" method is more promising, as it is believed to be less dependent on the grid size and the value of C_{SF} .



Fig. 7.18 The predicted surface emissive power using three different methods

7.4 MONTOIR 35 m POOL FIRE

7.4.1 Problem Descriptions

In this test [134], a 35 m diameter bund, made of a 100 mm thick layer of lightweight concrete, was built to retain the LNG. Prior to discharging LNG, a lightweight flammable cover was positioned 1 m above the bund floor to reduce the heat transfer due to solar radiation and convection between air and LNG. It is found that the steady methane fire period could be split into a series of shorter steady periods within which the wind conditions were relatively constant. The average value of mass burning rate was 0.14 kg/m²s. The average flame drag ratio, defined as the flame base length in the direction of the wind divided by the pool diameter, was measured to be around 1.29. The average flame length to pool diameter is estimated to be 2.24. It is worth pointing out that in the original experimental work [134] the flame length was defined as the distance from the centre of flame base (including flame drag) to the tip of the visible flame, while

in this study it is defined as the distance from the burner centre to that tip. In fact, 2.24 is a converted value based on our definition. The overall flame averaged SEP was measured to be in the range of $257 \sim 273 \text{ kW/m}^2$.

A cylindrical computational domain was set with the size of 300 m in diameter and 100 m in height, similarly to Fig. 7.11. Non-uniform meshes were also employed. The number of grid points across the burner was set as 40, 60 and 80 for "Coarse", "Medium" and "Fine" simulations, respectively. The magnitude of wind speed is 9.6 m/s in this scenario, obtained at 9 m above the ground in the test. The atmospheric velocity profile, i.e. Eq. (5.20), was applied to the cross wind inlet boundary similarly like Fig. 7.11, and the initial velocity field inside the domain was set as the same to improve numerical stability. The inlet mass flow rate is set as 134.70 kg/s according to the test, giving the theoretical heat release rate of 6780 MW. The integral length scale is calculated to be 32.73 m based on Eq. (2.28). Note that the temperature boundary condition for the gas methane inlet was set as fixed enthalpy flux rather fixed temperature, aiming to mimic temperature build-up over the inlet. Both turbulent Prandtl number and Schmidt number were set as 0.8. The physical time was set as 50 s to ensure the fire is fully developed, while the averaging process starts from 25 s after ignition. All the above settings are summarized in Table 7.3.

Table 7.3 Summary of	f numerical s	ettings for the	Montoir 35	m LNG fire
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Location	Montoir	
Fuel	Methane	
Smoke Point Height	0.29 m	
Fire Size	35 m	
Mass Flow Rate	134.70 kg/s	
Theoretical HRR	6780 MW	

Computational Domain	300 m (D) × 100 m (H)	
Mesh	Non-uniform grids; Cells across burner: Coarse, 40; Medium, 60; Fine, 80	
Fuel Inlet Temperature	Fixed enthalpy flux	
Wind Inlet Velocity	Atmospheric velocity profile	
LES Model	Sub-grid kinetic energy equation $C_c = 0.4$ $C_t = 0.05$	
Radiation Model	Finite volume method	
Soot Model	On	
Prandtl Number	0.8	
Lewis Number	1.0	
Integral Length Scale	32.73 m	
Physical Time	75 s	

7.4.2 Results and Discussions

a. Grid Sensitivity

The calculated flame height with the variation of grid size is demonstrated in Fig. 7.19. It is also observed that both the fluctuation of the flame height and its average value are increased, when the mesh changes from "Coarse" to "Medium". In contrast, "Fine" and "Medium" meshes produce very similar results, demonstrating that the grid size is getting independent. The average flame height in "Fine" simulation is predicted to be 43 m. Moreover, the variation of grid size has slight effect on the predicted flame tilted angle from the vertical direction, as found in Fig. 7.20. The time-averaged angle is simulated to be 57.0°. Combing with the flame angle and flame height, one could work out the averaged flame length, which is expressed as 43 m/cos57.0°, i.e. 79.0 m.

Therefore, the ratio of flame length to the burner diameter is calculated to be 2.26, quite close to the measurement of 2.24.



Fig. 7.19 The predicted flame height with different grid size



Fig. 7.20 The predicted flame angle with different grid size

b. Soot Formation Coefficient

The predicted soot yield with two formation coefficients is shown in Fig. 7.21. It is found that the transient value generally varies from 0.32 to 0.43, if the coefficient, i.e. 1.5E-5, achieved from smoke point height is employed. This prediction is thought to be approximately 2.3~3.1 times bigger than the preliminary estimation by Raj [138], i.e. 0.137. In contrast, the coefficient of 3.0E-6, tuned from the 14 m LNG fire scenario, could produce the average soot yield of 0.12, in reasonable agreement with that Raj's estimation. The impact of that tuned coefficient on the soot volume fraction and temperature is examined in Figs. 7.22 and 7.23. It is still clear that the transient and average soot volume fraction are generally decreased by nearly 4~6 times. The predicted average value with the coefficient of 3.0E-6 possesses the order of magnitude of 0.1 ppm. consistent with Raj's empirical estimation of 0.2 ppm [138]. From the profiles of average soot volume fraction, one could also observe that the flame is dragged out of the burner with the distance of around 17.5 m. Hence, the flame drag ratio is predicted to be around 1.5, a bit larger than the measurement of 1.29. It is depicted in Fig. 7.23 that the larger flame zone is achieved if the soot formation coefficient is decreased, which is associated with the fact that more energy is artificially released from the soot potential energy.



Fig. 7.21 The predicted soot yield with different soot formation coefficient



Fig. 7.22 The predicted transient and average soot volume fraction (ppm) with different soot formation coefficient (Row 1: $A_f/L_{sp} = 1.5E - 5$; Row 2:

 $A_f/L_{sp} = 3E - 6$; dash-dot line: burner rim)



Fig. 7.23 The predicted average temperature (K) with different soot formation coefficient ((a): $A_r/L_{ip} = 1.5E - 5$; (b): $A_r/L_{ip} = 3E - 6$; dash-dot line: burner rim)

c. Conservation of Energy

The predicted heat release rate, soot potential energy and total energy against time are displayed in Fig. 7.24. Bear in mind that the coefficient of 3.0E-6 is applied. It is found that around 819 MW of energy is stored in the soot particles, and the released energy from gas phase combustion and soot oxidation is approximated to be 6082 MW. Thus the total energy would be 6901 MW, which agrees reasonably with the theoretical value obtained from the inlet mass flow rate, i.e. 6780 MW.



Fig. 7.24 The predicted energy curves against time

d. Surface Emissive Power

The predicted surface emissive power applying three different methods is depicted in Fig. 7.25. The "Flame Emissivity" method predicts the average SEP of 233 kW/m², in reasonable agreement with the experimental data, i.e. 257~273 kW/m². As stated before, the "Surface Emissivity" method delivers relatively low magnitude of SEP, with the average value of 171 kW/m². The prediction with "Surface Heat Flux" is somewhere in-between, i.e. 197 kW/m². Therefore, it is established again that the "Flame Emissivity" method is more promising. Additionally, the predicted flame temperature is approximately 1424 K, while the absorption coefficient is estimated to be 3.3.



Fig. 7.25 The predicted surface emissive power using different methods

7.5 PHOENIX 56 m POOL FIRE

7.5.1 Problem Descriptions

In this test [136], about 198.5 m³ LNG was discharged through three discharge pipes. The average flow rate during the fully open period of 90 s was 1.91 ± 0.84 m³/s, yielding a mass discharge rate of 802 kg/s. The average wind speed was 1.6 m/s. The spreading LNG pool area continuously increased during the discharge interval, achieving an equivalent circular diameter of 81 m at the end of the spill. The burning rate could not be calculated, as the reservoir emptied prior to the pool achieving a constant area. It was unexpected that the fire did not attach to the leading edge of the spill, and hence the effective fire diameter was smaller than the spreading LNG pool diameter. The average flame width at 15 m above the pool was around 56 m and the average flame height was 146 m during the steady-state interval. The overall flame average SEP was measured to be 286 ± 10 kW/m².

A cylindrical computational domain was set with the size of 300 m in diameter and 300 m in height, analogously to Fig. 7.11. Non-uniform meshes were also employed, similarly like Fig. 6.2. The number of grid points across the burner of 56 m was selected to be 40, 60 and 80 for "Coarse", "Medium" and "Fine" simulations, respectively. The atmospheric velocity profile, i.e. Eq. (5.20), was applied to the cross wind inlet boundary similarly like Fig. 7.11, and the initial velocity field inside the domain was set as the same to improve numerical stability. As the fuel burning rate is not known in this test, the value should thus be pre-described before the simulation. In this study, 0.32 kg/m²/s is chosen, which is obtained from the measured discharging rate divided by the pool area,

and this number is expected to be the maximum value of burning rate for this scenario. Correspondingly, the theoretical heat release rate is calculated to be 39433 MW, while the integral length scale is calculated to be 66.82 m based on Eq. (2.28). The inlet temperature is set as 373 K considering the boiling of water during the burning. Both turbulent Prandtl number and Schmidt number were set as 0.8. The physical time was set as 100 s to ensure the fire is fully developed. All the above settings are summarized in Table 7.4.

Location	Phoenix		
Fuel	Methane		
Smoke Point Height	0.29 m		
Fire Size	56 m		
Mass Flow Rate	0.32 kg/m ² /s		
Theoretical HRR	39433 MW		
Computational Domain	300 m (D) × 300 m (H)		
	Non-uniform grids;		
Mesh	Cells across burner: Coarse, 40; Medium,		
	60; Fine, 80		
Fuel Inlet	373 K		
Temperature			
Wind Inlet Velocity	Atmospheric velocity profile		
	Sub-grid kinetic energy equation		
LES Model	$C_{\varepsilon} = 0.4$		
	$C_{k} = 0.05$		
Radiation Model	Finite volume method		
Soot Model	On		
Prandtl Number	0.8		
Lewis Number	1.0		
Integral Length Scale	66.82 m		
Physical Time	100 s		

Table 7.4 Summary of numerical settings for the Phoenix 56 m LNG fire

7.5.2 Results and Discussions

a. Grid Sensitivity

The calculated flame height with the variation of grid size is demonstrated in Fig. 7.26. It is found that the average flame height decreased against time up to 60 s and then maintained quasi-steady state. The reason is that fuel would strongly mix with air after entering the inlet boundary, resulting in the intensive combustion, particularly at the upper location of the flame. Therefore, one could find that the flame height is relatively larger during the first few puffing cycles. It is also observed that both the fluctuation of the flame height and its average value are increased, when the mesh varies from "Coarse" to "Medium". In contrast, "Fine" and "Medium" meshes produce very similar results, demonstrating that the grid size is getting independent. The average flame height in "Fine" simulation is predicted to be 72.4 m at the quasi-steady state. Moreover, the variation of grid size has slight effect on the predicted flame tilted angle from the vertical direction, as found in Fig. 7.27. It is also found that the average flame angle increase with time till around 65 s, and then tends to be quasi-steady with the value of around 65.2°. The reason is most likely to be associated with the strong air entrainment. This value is believed to be larger than the experimental finding, although no detailed measurement was made during the test. Combing with the flame angle and flame height, the average flame length is calculated to be 170.4 m, which is expressed as 72.4 m/cos65.0°. This predicted flame length is greater than the measured value of 146 m, and their difference must be related to the setting of maximum mass flow rate, as the exact value was not measured.



Fig. 7.26 The predicted flame height with different grid size



Fig. 7.27 The predicted flame angle with different grid size

b. Conservation of Energy

The predicted heat release rate, soot potential energy and total energy against time are demonstrated in Fig. 7.28. Note that the coefficient of 3.0E-6 is applied. It is observed that around 7171 MW of energy is stored into soot

particles, and the released energy from gas phase combustion and soot oxidation is approximated to be 34785 MW. Thus the total energy would be 41956 MW, with the discrepancy of around 6 % by comparing with the theoretical value obtained from the inlet mass flow rate, i.e. 39433 MW. This discrepancy may also be related to the setting of maximum mass flow rate, which may not be reached for the real fire with this kind of scale. Unfortunately, it is impossible to verify it, as no relevant measurement was reported.



Fig. 7.28 The predicted energy curves against time

c. Surface Emissive Power

The predicted surface emissive power applying three different methods is depicted in Fig. 7.29. The "Flame Emissivity" method predicts the average SEP of 346 kW/m², in reasonable agreement with the experimental data, i.e. 286 ± 10 kW/m². The discrepancy is expected to be associated with the setting of maximum mass flow rate, resulting in more energy released from the combustion and soot oxidation. As stated before, the "Surface Emissivity" method and "Surface Heat Flux" method deliver relatively low magnitude of SEP, with the average value of 253 kW/m² and 247 kW/m², respectively. According to the fact that the maximum value was set for the mass flow rate, the SEP is believed to be over-predicted, and the "Flame Emissivity" method is thus more promising, as established before.



Fig. 7.29 The predicted surface emissive power using different methods

d. Temperature and Soot Volume Fraction

The predicted transient (at 100 s) temperature and soot volume fraction is shown in Fig. 7.30. It is seen that the flame is dragged out of the burner near the fire base, due to the existence of cross wind. The dragging distance is estimated to be around 57 m from the temperature profile, provided that the critical flame temperature is set as 1000 K. One can also find that the flame on the "upwind" side becomes more turbulent than that on the "downwind" side, and this should be attributed to the interaction between the flame and the cross wind. The transient temperature is simulated be less than 1800 K in the majority of the flame. From the soot volume fraction profile, one can observe that the soot particles can escape from the flame, indicating the role of turbulence in the soot transport. The magnitude of soot volume fraction is calculated to be less than 3.0 ppm.



Fig. 7.30 The predicted transient (at 100 s) temperature (K) and soot volume fraction (ppm) profiles



Chapter 8

Conclusions and Future Work

8.1 CONCLUSIONS

A comprehensive combustion and soot modelling approach in the LES frame for fire simulations has been developed. The procedures have also been developed to calculate the flame height, flame angle, radiative fraction, flame angle and surface emissive power. These models and approaches have been implemented into the FireFOAM solver. A series of fire scenarios with different fuels, including methanol, methane, heptane, and toluene, and with different sizes ranging from 30 cm to 56 m, have been performed for their validation and application studies. The major conclusions are summarized as follows.

8.1.1 Eddy Dissipation Concept

The original turbulent energy cascade of EDC is extended to the LES framework, assuming that there is always a structure level at which the typical length scale is equivalent to the filter width of LES. Since the velocity scale at that structure level could be estimated from the SGS kinetic energy, all other quantities would thus be calculated at this structure level according to the general formulations in the original turbulent energy cascade. Based on this known structure level, the total kinetic energy and dissipation rate would be estimated, provided that the integral length scale is assumed to be equivalent to the

characteristic length of fire plume. Hence, the time scales, such as Kolmogorov time scale and integral time scale, would be calculated, which are important for the soot model development.

A 30.5 cm methanol fire was conducted to verify this combustion model, as fuel methanol is very clean and then soot model is not activated. First of all, the grid sensitivity study has been conducted to ensure the grid size is adequate, based on the curves of axial mean temperature and velocity against the grid size. as well as the profiles of temperature and velocity fluctuations with the variation of grid size. The new formulations of γ and χ have been examined, regarding the different initial conditions and different ignition methods, and the new χ formulation has been found to be able to tackle the lifted problem due to the original one. The heat release rate, radiative fraction, velocity and its fluctuation, temperature and its fluctuation, turbulent heat flux, SGS and total dissipation rate, SGS and total kinetic energy, time scales, and length scales have been compared with the corresponding experimental data, and reasonable agreement has been observed, suggesting that the extended EDC in this study is promising. It is worth mentioning that Kolmogorov time scale and integral time scale have been captured within the same order of magnitude as the measurement, which is really encouraging in the LES of fire dynamics, and this conclusion would give us more confidence for the soot model development.

8.1.2 Smoke Point Soot Model

In laminar flames the instantaneous soot mass fraction transport equation would be solved, while it is not applicable to the turbulent flames, as the turbulent fluctuations play a very important role. After the filtering process and

the conversion of mixture fraction, the instantaneous transport equation would be transformed to the one for the filtered soot mass fraction. By neglecting the thermophoresis term and modeling the unresolved scalar flux and the soot diffusion term, one would thus realize that the key issue for this extension would be how to treat the filtered soot source terms, including the soot formation and oxidation processes. In this study, the filtered soot formation rate has been accounted for using the concept of PaSR, and this rate is thus linked to the laminar based soot formation rate substituted with the filtered properties, through the formulation of κ . Note that in κ the soot formation chemical time scale has been assumed to be proportional to the SPH while its turbulent mixing time has been supposed to be the geometric mean of the Kolmogorov time scale and integral time scale. In contrast, the filtered soot oxidation rate has been considered by imitating the gas phase combustion model, i.e. EDC, as the soot particles are assumed to be the solid phase of the fuel. Hence, the soot oxidation chemical time scale has been implicitly set to be infinitely fast. Moreover, the corresponding mixing time scale for soot oxidation has been chosen to be the same as the soot formation. The roadmaps of soot formation and oxidation have also been developed in order to account for the effect of soot on the fuel distribution and energy transport.

A series of fire scenarios with different fuels, including methane, heptane, and toluene, have been investigated to validate the coupling between the extended EDC and SPSM. These fuels represent three different levels of soot production, i.e. light, moderate, and heavy. The grid sensitivity study has been performed for each scenario by comparing the curves of axial mean temperature and velocity against the grid size, and also considering the profiles of temperature and velocity fluctuations with the variation of grid size. The sensitivity study has also been conducted for the radiative properties, such as the number of solid angles and solving frequency of RTE. The new expression of χ has been proved again to be capable of tackling the non-physical lifted problem. The relationship between the soot formation chemical time scale and mixing time scale has been investigated, as well as its effect on κ . The typical distributions for the soot formation rate, oxidation rate, and net soot production rate have been discussed. The conservation of total energy, including heat release rate and soot potential energy has been examined to ensure that the unexpected energy loss is negligible. The flame height, radiative fraction, soot volume fraction and its fluctuation, and temperature and its fluctuation have been compared with the corresponding experimental data, and reasonable agreement has been observed, suggesting the current coupling of the extended EDC and SPSM is encouraging in the LES of fire dynamics.

8.1.3 Others

The method to calculate the flame height in the sooty flames has been developed and then verified in the current study. The approach to obtain the radiative fraction has also been considered by integrating the radiation source term in the energy transport equation over the entire flame envelope, and then validated in the non-sooty and sooty flames. Three different methods have been developed to estimate the SEP, which is one of the most important quantities in the large scale LNG pool fires, and it has been observed that the "Flame Emissivity" method could give relatively better predictions, which is recommended in this study. The coupling of the extended EDC and SPSM, as well as the approaches to calculate the flame height, radiative fraction and SEP, have been further applied to the large scale LNG pool fires. Reasonable agreement between the predictions and measurements further demonstrates the capability of models mentioned above, in spite of the huge length scales involved. Note that the pre-exponential coefficient A_f/L_{sp} in the filtered soot formation rate has been artificially tuned from the default value of 1.5E-5 to 3E-6 in the large scale LNG pool fires, as it has been found that the coefficient of 1.5E-5 may have hugely over-predicted the soot production, in comparison with other researchers' studies.

8.2 FUTURE WORK

Although the reasonable agreement between predictions and measurements has been achieved for the small, medium, and large scale fire scenarios, there is still room to further enhance the combustion and soot models.

8.2.1 Eddy Dissipation Concept

The concept of the turbulent energy cascade, which is the foundation of EDC, may face challenges in practice. In this study, the turbulent energy is always assumed to transfer from the large scales to the small scales, while the backscatter and upscale transfer phenomena would take place in real physics. In fact, the fraction of energy due to the backscatter and upscale transfer needs to be understood. This fraction might be relatively small, and thus one may regard the current turbulent energy cascade model has taken into account the net energy transfer.

It is known that the drive of the fire is buoyancy rather than momentum, and thus the effect of buoyancy on the turbulent energy transfer and even on the reaction rate in EDC needs to be investigated. Regarding this issue, we can hardly rely on experimental approach because of micro-scales of turbulent structures, and then theoretical analysis may play a dominant role.

8.2.2 Smoke Point Soot Model

It is concluded that the expression of κ , i.e. Eq. (3.15), has the great effect on the filtered soot formation rate in LES, further on the soot volume fraction. Thus the estimation of the chemical time scale and of the turbulent mixing time scale for soot formation is of extreme importance. In this work, the soot formation chemical time scale is assumed to be proportional to the laminar smoke point height, and the fuel-independent coefficient was estimated based on the soot formation residence time of 40 ms for the laminar ethylene flame. This assumption should be further verified based on the more detailed experimental studies for a variety of fuels. Furthermore, the soot formation chemical time scale may be affected by the local turbulent mixing in the reacting zone of PaSR, and thus the expression of κ may be further improved.

The turbulent mixing time scale for soot formation is estimated from the Kolmogorov time scale and the integral time scale, as the corresponding structure level on which the soot formation process takes place is unknown to us in the turbulent energy cascade of EDC. More works can be done to improve the prediction of this mixing time scale, as well as the sensitivity study due to the different expressions.

8.2.3 Others

As mentioned in Chapter 5, the non-physical pressure and velocity would be obtained in the fire scenarios with the cross wind, if no special treatment is performed to the original FireFOAM. In this work, the issue is bypassed by neglecting the Dp/Dt term in the energy transport equation, similar to the treatment in the low Mach number assumption. Fundamentally, the reason for this problem is due to lack of the appropriate boundary conditions for the pressure and velocity in the compressible solver, which are not included in the existing OpenFOAM. One might have a try to implement the more advanced Navier Stokes characteristic boundary conditions to tackle this issue. Furthermore, this settlement will also benefit the numerical simulation of a compartment fire.

Importantly, more experimental studies should be carried out, as the number of fire scenarios, which are useful for the soot model validation, is really limited, particularly for the moderately and heavily sooty fires. Moreover, the possible over-prediction of soot production in the large scale LNG pool fires has suggested that the application of the current models to the large scale fires would face more challenges, especially for the heavily soot fires.

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