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Abstract

Turbulent combustion is a primary phenomena determining the performance of practical applications such as furnace, disel engines, gas turbine engines, and many aerospace devices include rockets. For developing high-performance devices, understanding flame characteristics of turbulent combustion in a device is required, typically in a respect of combustion efficiency, stability, and pollutant emissions. With a development of turbulent schemes, called large eddy simulation (LES), with dynamic subgrid models and the rapid advances in computer technology, the significant progress on computational research for turbulent combustion has been achieved in recent decades. Especially, LES with flamelet approach has been found as a one of adaptive options for device-scale simulations due to its significant reduction of computational cost and feasibility to implement as an extension to conventional codes for non-reacting flows. In this study, LES solver using flamelet combustion models (steady laminar flamelet model (SLFM) and flamelet progress variable approach (FPVA)) is developed on open-source frameworks. For the code development, related theories on combustion and turbulent models are reviewed first. Detail descriptions of the developed codes are presented from the flamelet generation process to the LES solver. Finally, validation of the new solver is conducted with the partially premixed jet flame (Sandia D). The generated flamelet library and LES results show good agreement with the experimental data.

Keywords: LES, Flamelet Model, Turbulent Flame, Simulation, Sandia D
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1.1 Introduction

Combustion is the primary method to get energy from natural resources. In practical applications such as furnace, disel engines, and aircraft gas turbine engines, turbulence of flow interacts with combustion, which is called turbulent combustion. Turbulent combustion is a complicated phenomenon in that it involves various time and length scales, and the interaction of turbulence and the flame occurs in two-ways: turbulence enhances the chemical reaction in general and the heat release from the combustion alters the turbulence. For developing high-performance engines, understanding flame characteristics such as combustion efficiency, stability, and pollutant emissions is required. For that purpose, experimental research has been conducted mainly for turbulent combustion fields for several decades. Recently, as numerical modeling capability has been matured rapidly along with the advance of the performance of computational facilities, computational research on turbulent combustion with a
certain combustion modeling has become a viable approach for practical combustion devices.

![Figure 1.1 Turbulent combustion and thermo-acoustic instability in an annular combustion chamber](image)

**Computational approaches for turbulent combustion**

In direct numerical simulation (DNS) for turbulent combustion, without turbulent and combustion models, extreme computational cost is required to resolve both space and time. Unlike the conventional DNS for non-reacting flows, the time and length scales are not only bounded by the Kolmogorov scales, but also governed by those scales involved in chemical reactions. Even at the low Reynolds number regime, the required spatial resolution is typically order of 10 micrometers, which is translated to a billion grid points for a 1 cm³ cube computational domain. It is intractable to apply DNS on practical-scale applications, especially when the Reynolds number becomes larger.
On the other hand, for combustion simulations, exceedingly large simulation cost also arises from solving all transport equations of detail species. For example, 53 species and 325 reactions are involved in detailed GRI-Mech 3.0 chemical mechanism. For practical fuels other than Methane, the mechanism gets much larger as the carbon number increases. Some modern kinetics mechanisms of alternative fuels deal with several thousands of species.

Figure 1.2 Turbulent kinetic energy spectrum

Instead of direct numerical simulation (DNS), large-eddy simulation (LES) which solves a fraction of inertial subrange directly has been introduced to combustion community for practical-level applications. In LES, large-scale turbulence motions which are larger energy-containing level are directly resolved, while subgrid (or subfilter) scale turbulence motions and the effects of small-scale motion are modelled. With the scale separation concept of LES, lower resolution quality is achieved compared to DNS which requires extremely high resolution as same order of Kolmogorov eddy scale $\eta$. Compared with Reynolds
averaging Navier-Stokes simulation (RANS), much accurate turbulent flow field can be acquired because energy containing integral scales, which was modelled in RANS, are solved directly in LES. However, the advantage of scale separation concept of LES becomes not evident when it comes to reactive flows. Chemical reaction occurs on molecular level, where reactants are mixed enough and chemical reaction can happen. Even if resolution is enough for turbulent scale, the filter size of LES cannot be equal to molecular level. Therefore, a certain combustion model which can be used with LES to model subgrid turbulent-combustion interaction is needed. Various combustion models with LES to simulate turbulent combustion have been developed and studied in recent decades.

Combustion models for turbulent combustion

Various turbulent combustion models have been used in practice, such as transported probability density function (TPDF) [2, 3, 4], conditional moment closure (CMC) [5, 6], linear eddy modeling [7, 8], and flamelet approach [9, 10, 11, 12, 13, 14, 15]. Among these models, the flamelet approach has become one of viable options for device-scale simulations due to its significant reduction of computational cost and feasibility to implement as an extension to conventional codes for non-reacting flows.

1.2 Goal

The purpose of the present study is two-fold: One is to obtain an overview of available methods of LES with flamelet combustion model. The other is to develop an LES solver with flamelet approach which can simulate turbulent combustion. The developed solver is validated with a canonical piloted non-premixed flame, called Sandia flame D, to show validity and feasibility of the
developed code. In this study, a particular effort has been put on developing all relevant tools and solvers based on open-source libraries, to maximize the usage of the developed framework in the community and to welcome collaborative contribution from the community.

1.3 Outline

The contents of this thesis are organized as follows:

In chapter 1, details of flamelet combustion models are introduced. First of all, concept and assumptions of flamelet combustion model are introduced. Next, two important versions of flamelet models are discussed in detail. One is the original version of flamelet approach, steady laminar flamelet model (SLFM), suggested by Peters [9]. The other is an improved version, flamelet progress variable approach (FPVA), developed by Pierce and Moin [11]. With the discussion of two flamelet models, principal quantities for flamelet combustion model such as mixture fraction \((Z)\), scalar dissipation rate \((\chi)\), and progress variable \((C)\) are described together.

In chapter 2, the system of governing equations of LES with flamelet model is described. Starting from conventional governing equations for reactive flows, additional governing equations for flamelet combustion model are introduced. For the next, the filtered governing equations for LES are derived from the conventional governing equations applying the principal concept of LES, the scale-seperation concept. Induced closure problem and some subgrid models to close the system are explained. Finally, the closed system of filtered governing equations for LES with flamelet combustion model is derived.

In chapter 3, details of developed codes are described and categorized into two parts. First part is a describing of processes needed to generate flamelet
libraries, consists of the calculation of one-dimensional laminar flamelet solution and the pdf integration. Second part is a describing of solver to solve entire system of governing equations for LES with flamelet combustion models. The developments of codes are all based on open-source modules (Cantera, Ember, OpenFOAM) and short introduction of these modules are also included.

In chapter 4, validations for our new developed codes are conducted. Partially premixed jet flame, Sandia flame D, is chosen as a validation case. Apriori study to validate generated flamelet library and LES simulation is conducted. Details of simulation and the simulation results compared with experiment data of Sadia flame D are described.
In this chapter, details of flamelet combustion models are discussed. First of all, concept and assumptions of flamelet combustion model are introduced. Next, two important versions of flamelet models are discussed in detail. One is the original version of flamelet approach, steady laminar flamelet model (SLFM), suggested by Peters [9]. The other is an improved version, flamelet progress variable approach (FPVA), developed by Pierce and Moin [11]. With the discussion of two flamelet models, principal quantities for flamelet combustion model such as mixture fraction ($Z$), scalar dissipation rate ($\chi$), and progress variable ($C$) are described together.

### 2.1 Background

Flamelets are thin reactive-diffusive layers embedded within non-reacting turbulent flow field [16]. If the chemical time scale is small enough compare to the flow time scale, we can assume that reactions occur in a thin layer around
stoichiometric mixture on a scale smaller than the Kolmogorov eddy. With this assumption, structures of the reactive zone trace laminar flamelets.

With the concept, in flamelet combustion model, turbulence-combustion interaction and detailed chemistry can be mapped by several representative parameters on laminar flamelet database, instead of solving directly entire species equations. The flamelet approach for non-premixed flames, which views a turbulent flame as an ensemble of laminar flamelets, was first suggested by Peters [9]. Afterward, various modified versions of flamelet approach has been suggested and applied for the simulation of turbulent combustion [10, 11, 12, 13, 14, 15].

**Figure 2.1 Evolution of flamelet approaches**

In general, these various versions of flamelet combustion models can be categorized into two group by the choice of the representative parameter on which flamelet database is generated and parameterized for non-equilibrium effect. One uses scalar dissipation rate [9, 10], based on steady laminar flamelet model (SLFM) suggested by Peters, and the other uses progress variable [11,
12, 13, 14, 15], based on flamelet progress variable approach (FPVA) modified by Pierce and Moin, as the representative parameter.

2.2 Steady laminar flamelet model (SLFM)

The steady laminar flamelet model (SLFM) focuses on the location of the flame surface and not on the reactive scalars themselves [16]. A Flamelet library which contains reactive scalars and thermodynamic information, such as temperature, mass fraction of reactive species, and diffusion coefficients, is parameterized by some representative parameters which fully determine the state of reaction on each cells. In SLFM, filtered mixture fraction ($\tilde{Z}$) and filtered scalar dissipation rates ($\tilde{\chi}$) are considered as essential flamelet parameters, and filtered subgrid variance of mixture fraction ($\tilde{Z}'^2$) is normally used as a flamelet parameter to imply adaptive turbulent-combustion interactions on subgrid scale. In here, only the definitions and roles of representative parameters itself without filtering (mixture fraction $Z$ and scalar dissipation rate $\chi$) will be discussed, and the filtered function and the subgrid variance of scalar fluctuation will be discussed separately on next chapter.

**Mixture fraction**

Mixture fraction $Z$ (also denoted by $f$ or $\xi$) is a principle quantity in non-premixed combustion. The value describes how much fuel and oxidizer mixed in a typical location, between 0 and 1 (0 denotes oxidizer state, 1 denotes fuel state). Various definition of mixture fraction can be conceived by focusing on which reactive species used on definition. For a same mixture condition, the value of mixture fraction at a certain location may be different across these various definitions because of the difference between diffusivity of each chemical
species, i.e., due to the differential diffusion effect.

In case Hydrocarbon \((C_mH_n)\) is used for fuel, the global reaction equation for complete combustion is written as

\[
C_mH_n + (m + \frac{n}{4})O_2 \rightarrow mCO_2 + \frac{n}{2}H_2O
\]  

(2.1)

Bilger [17] defined a mixture fraction on C, H, and O elements, which reads as follows:

\[
Z = \frac{Z_C/(mW_C) + Z_H/(nW_H) + 2(YO_2,2 - Z_O)/((m + \frac{n}{4})WO_2)}{Z_{C,1}/(mW_C) + Z_{H,1}/(nW_H) + 2YO_2,2/((m + \frac{n}{4})WO_2)}
\]  

(2.2)

Barlow modified Bilger’s definition by removing oxygen terms, in order to make the mixture fraction less sensitive to experimental noise and interference from laser-induced fluorescence [18].

According to Barlow’s definition [18], the mixture fraction can be written as:

\[
Z = \frac{Z_C/(mW_C) + Z_H/(nW_H)}{Z_{C,1}/(mW_C) + Z_{H,1}/(nW_H)}
\]  

(2.3)

Mixture fraction plays most important roles on flamelet combustion model for non-premixed flame as determines the location of flamelet. At the location of stoichiometric mixture fraction \((Z_{st})\), where reactants mixed on stoichiometric conditions, most reactive and highest temperature will exist. At the location of 0 or 1 mixture fraction, non-reacting flow exist because there are only reactants or products state. Therefore, in SLFM, the field of mixture fraction is solved for determining the reactiveness on each location. When generating non-premixed flamelet database, if the solution of a one-dimensional laminar flame is obtained in the physical domain, it needs to be transformed to the mixture fraction domain following one of the mixture fraction definitions described above.
Scalar dissipation rate

Scalar dissipation rate ($\chi$) is another principal parameter in SLFM. Instantaneous scalar dissipation rate defined as

$$\chi = 2D|\nabla Z|^2 \quad (2.4)$$

It has the dimension of an inverse time and represents the inverse of a diffusion time scale. It also can be thought as a diffusivity in mixture fraction space [16] and gives non-equilibrium effects on flamelet. If turbulent flow strains reaction region, the gradient of mixture fraction ($\nabla Z$) will be increased, and finally increasing scalar dissipation rate.

Limitations of SLFM

In SLFM, non-equilibrium effect of flamelet solution is parameterized by scalar dissipation rate. Figure (2.3) shows the maximum temperature of steady flamelet solutions as a function of the scalar dissipation rate ($\chi$), which can be called ‘S-curve’. As scalar dissipation rate increases, strain rate of each laminar flame increases and maximum temperature gets lower. At a critical point, flame cannot
continue reaction and non-reactive (extinction) solution is obtained. Between the critical point and extinction stage, transient unstable branch may exist. Therefore, multiple solutions (steady and transient solutions) can be found on a single scalar dissipation rate value. As a result, by means of scalar dissipation rate, entire transient flamelet solutions cannot be included in SLFM as shown in figure (2.4).

In SLFM flamelet libraries, discontinuous jump of the flamelet solution is unavoidable near the critical scalar dissipation rate. This also may give rise to instability in the numerical simulation itself.

2.3 Flamelet progress variable approach (FPVA)

Pierce & Moin [11] suggested flamelet progress variable approach (FPVA) to overcome limitations of SLFM described above. Instead of scalar dissipation rate ($\chi$) implying non-equilibrium effect, specially defined progress variable is used as an essential flamelet parameter. Then, a flamelet library which contains reactive scalars and thermodynamic information, such as temperature, mass fraction of reactive species, and diffusion coefficients, are parameterized essentially by filtered mixture fraction ($\tilde{Z}$) and filtered progress variable ($\tilde{C}$), optionally by filtered subgrid variance of scalars ($\tilde{Z}''^2$, $\tilde{C}''^2$) which fully determine the state of reaction on each cells. With the use of progress variable, flamelet libraries can include transient solutions on re-ignition and extinction stage. Similar to SLFM, in here, only the definitions and roles of progress variable ($C$) itself without filtering will be discussed, and the filtered function and the subgrid variance of scalar fluctuation will be discussed separately on next chapter.
Figure 2.3 Locus of maximum flame temperatures from a complete set of steady-flamelet solutions including the unstable branch. [11]

Figure 2.4 Locus of maximum flame temperatures in SLFM. [11]
Progress variable

Progress variable (generically denoted by $C$) is a reactive scalar which tracks the global extent of reaction of the local mixture [11], 0 denotes mixtures of reactants and maximum value ($C_{\text{max}}$) denotes mixtures of products. Various definition of progress variable can be selected. The reduced temperature is one of options [12],

$$C = \frac{T - T_{st,u}}{T_{st,c} - T_{st,u}}$$  \hspace{1cm} (2.5)

where, $T_{st,u}$ is the temperature at stoichiometric mixture fraction on unburnt flamelet solution, while $T_{st,c}$ is the temperature at stoichiometric mixture fraction on unstrained flamelet solution. The summation of typical species mass fraction ($Y_\alpha$) also can be selected as progress variable [11, 19] such as,

$$C = Y_{CO_2} + Y_{H_2O}$$  \hspace{1cm} (2.6)

$$C = Y_{CO_2} + Y_{CO} + Y_{H_2O} + Y_{H_2}$$  \hspace{1cm} (2.7)

The summation of typical species mass fraction ($Y_\alpha$) divided by molecular weight ($M$) of species is selected as progress variable ($C$) to ensure a monotonous increasing of progress variable ($C$) for all flamelets [20].

$$C = \frac{Y_{H_2}}{M_{H_2}} + \frac{Y_{H_2O}}{M_{H_2O}} + \frac{Y_{CO_2}}{M_{CO_2}}$$  \hspace{1cm} (2.8)

In flamelet combustion model, typically in FPVA, progress variable has the role of determining the state of reaction with mixture fraction. State of reaction can be different on the same state of mixing between fuel and oxidizer (on same mixture fraction value) because of the non-equilibrium influence on flamelet.
While progress variable ($C$) replaces the role of the scalar dissipation rate ($\chi$), it allows one to define the state of reaction between the critical points and the extinction (non-reacting) state, along the unstable branch or along the ignition or extinction path, which is not conceivable if one uses the scalar dissipation rate.
In this chapter, the system of governing equations of LES with flamelet model is described. Starting from conventional governing equations for reactive flows, additional governing equations for flamelet combustion model are introduced. For the next, the filtered governing equations for LES are derived from the conventional governing equations applying the principal concept of LES, the scale-separation concept. Induced closure problem and some subgrid models to close the system are explained. Finally, the closed system of filtered governing equations for LES with flamelet combustion model is derived.
3.1 Governing Equations for reactive flow

The conventional system of governing equations

The conventional system of governing equations for reactive flow without turbulence and combustion modelling consists of conservation equations for mass, momentum, energy, and species mass fractions. The conservation equations are written as

**continuity:**

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \tag{3.1}
\]

**momentum:**

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j + \delta_{ij} p)}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} = \rho g_i \tag{3.2}
\]

**energy:**

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial [(\rho E + p) u_j]}{\partial x_j} - \frac{\partial (\tau_{ij} u_i)}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = \rho g_i u_i \tag{3.3}
\]

**species mass fractions** \((\alpha = 1, \ldots, N):\)

\[
\frac{\partial (\rho Y_\alpha)}{\partial t} + \frac{\partial (\rho Y_\alpha u_j)}{\partial x_j} + \frac{\partial J_{j,\alpha}}{\partial x_j} = \dot{w}_\alpha \tag{3.4}
\]

where viscous stress tensor \((\tau_{ij})\), total heat flux \((q_j)\) which means energy flux due to thermal conduction and diffusion of species, and mass diffusivity flux corresponding to species \(\alpha (J_{j,\alpha})\) are

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_l}{\partial x_l}, \tag{3.5}
\]

\[
q_j = -\lambda \frac{\partial T}{\partial x_j} - \rho \sum_{\alpha=1}^{N} h_{\alpha} D_{\alpha} \frac{\partial Y_\alpha}{\partial x_j}, \tag{3.6}
\]

\[
J_{j,\alpha} = -\rho D_{\alpha} \frac{\partial Y_\alpha}{\partial x_j} \tag{3.7}
\]
\( \rho, u, p, E, Y_\alpha, T \) and \( h \) represent density, velocity, pressure, total energy, species mass fraction, temperature, and enthalpy of mixture. \( \dot{w}_\alpha \) represents the net rate of production of the species. \( \mu, \lambda, \) and \( D_\alpha \) denote viscosity, thermal conductivity, and molecular diffusivity of species \( \alpha \), respectively. \( \delta_{ij} \) is Kronecker delta.

With the system of conservation equations (Eqs. (3.1), (3.2), (3.3), and (3.4)), we only have total \( N+5 \) equations for total \( N+6 \) unknowns \((\rho, u_x, u_y, u_z, T, Y_1, \ldots, Y_N, \text{ and } p)\). Additionally, equation of state (EOS) for ideal gas is considered as a constitutive equation for solving the entire system.

\[
P = \rho RT
\]

### Additional governing equations required for flamelet combustion model

When using flamelet combustion models, additional governing equations are needed to close flamelet library parameters and the system of governing equations. In this study, flamelet library which contains all the chemical reaction quantities has two parameterized options,

with SLFM:

\[
\tilde{\phi}(\tilde{Z}, \tilde{Z}^\mu, \tilde{\chi})
\]

with FPVA:

\[
\tilde{\phi}(\tilde{Z}, \tilde{Z}^\mu, \tilde{C})
\]

In this study, filtered scalars \((\tilde{Z} \text{ and } \tilde{C})\) are acquired by solving the filtered transport equations for scalars (Eqs. (3.16) and (3.17)) which are derived in the previous section, while filtered subgrid variance of mixture fraction \((\tilde{Z}^\mu)\) and filtered scalar dissipation rate \((\tilde{\chi})\) are acquired by subgrid modelling. To derive the filtered transport equations for scalars (Eqs. (3.16) and (3.17)), scalar
transport equations for mixture fraction and progress variable is required and written as

scalar transport equation for mixture fraction:
\[
\frac{\partial (\rho Z)}{\partial t} + \frac{\partial (\rho u_i Z)}{\partial x_i} + \frac{\partial J_{J,Z}}{\partial x_j} = 0 \quad (3.9)
\]

scalar transport equation for progress variable:
\[
\frac{\partial (\rho C)}{\partial t} + \frac{\partial (\rho u_i C)}{\partial x_i} + \frac{\partial J_{J,C}}{\partial x_j} = \dot{w}_C \quad (3.10)
\]

where
\[
J_{J,Z} = -\rho D_Z \frac{\partial Z}{\partial x_i}, \quad (3.11)
\]
\[
J_{J,C} = -\rho D_C \frac{\partial C}{\partial x_i} \quad (3.12)
\]

\(D_Z\) and \(D_C\) denotes diffusivity of mixture fraction and progress variable. Diffusion coefficient of mixture fraction and progress variable \((D_Z\) and \(D_C\)) is rather arbitrary. According to Peters [16], thermal diffusivity is recommended for the diffusion coefficient of mixture fraction because diffusion of enthalpy is the most important transport process in mixture fraction space.

3.2 Filtered Governing Equations for LES

Principal concept of large-eddy simulation (LES) is a separation of turbulence scales. Large-scale turbulence motions which is a larger energy-containing level is directly computed, while small-scale turbulence motions and the effects of small-scale motion are modelled. Grid size is normally consumed as a filter size \((\Delta)\) which separate large and small scales as low-pass spatial filtering. With filtering, flow variables in LES system appear in the filtered (resolved) and the residual (subgrid-scale) quantities. Filtered governing equations for LES can be achieved by averaging the original system of governing equations. With
conventional averaging method (Reynolds averaging), Favre averaging method is widely used in variable density flow because of its considerable advantages in the simplification of filtering equations (density residual value $\rho''$ does not appear) [16].

**Favre averaging**

Favre averaging is an averaging method with density-weighted. We can split a scalar quantities, $\phi(x, t)$, into $\tilde{\phi}(x, t)$ and $\phi''(s, t)$ which satisfying $\rho\phi'' = 0$.

\[
\phi = \tilde{\phi} + \phi''
\]

\[
\rho\phi = \rho\tilde{\phi} + \rho\phi''
\]

Averaging quantities,

\[
\rho\tilde{\phi} = \rho\tilde{\phi} + \rho\phi''
\]

\[
\rho\phi'' = 0
\]

Finally, Favre averaging is defined as,

\[
\tilde{\phi} = \frac{\rho\phi}{\rho}
\]

(3.13)

**The system of filtered governing equations for LES**

The system of governing equations for flamelet combustion model consists of conservation equation for mass (3.1), conservation equation for momentum (3.2), transport equation for mixture fraction (3.9), and transport equation for progress variable (3.10). The LES formulations for flamelet combustion model are derived by filtering the system of governing equations.

continuity :

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \tilde{u}_j}{\partial x_j} = 0
\]

(3.14)
momentum:
\[
\frac{\partial \bar{\rho} \vec{u}_i}{\partial t} + \frac{\partial (\bar{\rho} \vec{u}_i \vec{u}_j + \delta_{ij} \rho)}{\partial x_j} - \frac{\tau_{ij}}{\partial x_j} = \bar{g}_i + \frac{\sigma_{ij}}{\partial x_j} + \frac{\partial (\tau_{ij} - \bar{\tau}_{ij})}{\partial x_j} \tag{3.15}
\]

scalar transport equation for mixture fraction:
\[
\frac{\partial (\bar{\rho} \bar{Z})}{\partial t} + \frac{\partial (\bar{\rho} \vec{u}_j \bar{Z})}{\partial x_j} + \frac{\partial \bar{J}_{j,Z}}{\partial x_j} = - \frac{\partial (\bar{\rho} \bar{u}_j \bar{Z}''')}{\partial x_j} - \frac{\partial (\bar{J}_{j,Z} - \bar{J}_{j,Z})}{\partial x_j} \tag{3.16}
\]

scalar transport equation for progress variable:
\[
\frac{\partial (\bar{p} \bar{C})}{\partial t} + \frac{\partial (\bar{p} \vec{u}_j \bar{C})}{\partial x_j} + \frac{\partial \bar{J}_{j,C}}{\partial x_j} = - \frac{\partial (\bar{p} \bar{u}_j \bar{C}''')}{\partial x_j} - \frac{\partial (\bar{J}_{j,C} - \bar{J}_{j,C})}{\partial x_j} + \bar{w}_C \tag{3.17}
\]

Bar $\bar{}$ and tilde $\tilde{}$ symbols denote filtered quantities, former is with Reynolds averaging and the latter is with Favre averaging. Check $\check{}$ denotes quantities that are calculated from filtered values achieved in LES, for example,
\[
\check{\tau}_{ij} = 2 \check{\mu}(\check{S}_{ij} - \frac{1}{3} \delta_{ij} \check{S}_{ll}) \tag{3.18}
\]
\[
\check{J}_{j,Z} = - \check{D}_Z \frac{\partial \check{Z}}{\partial x_j} \tag{3.19}
\]
\[
\check{J}_{j,C} = - \check{D}_C \frac{\partial \check{C}}{\partial x_j} \tag{3.20}
\]

where,
\[
\check{\mu} = \mu(\check{T})
\]
\[
\check{S}_{ij} = \frac{1}{2} \left( \frac{\partial \vec{u}_i}{\partial x_j} + \frac{\partial \vec{u}_j}{\partial x_i} \right)
\]
\[
\check{D}_Z = D_Z(\check{T})
\]
\[
\check{D}_C = D_C(\check{T})
\]

$\check{S}_{ij}$ denotes strain rate tensor corresponding to the Favre-filtered velocity. Viscosity $\check{\mu}$ and diffusivities $\check{D}$ are tabulated on flamelet library which is achieved with the Favre-filtered temperature $\check{T}$. 

21
Closure problems and assumptions

The system of filtered governing equations for LES with flamelet combustion model (Eqs. (3.14), (3.15), (3.16), and (3.17)) includes several unclosed terms (I, II, III, IV, V, VI). With assumptions that the difference between filtered and calculated value of viscous stress tensor ($\tau_{ij}$) and diffusivity flux ($J_{j,Z}$, $J_{j,C}$) can be ignored,

\[ \tau_{ij} = \tilde{\tau}_{ij} \]
\[ J_{j,Z} = \tilde{J}_{j,Z} \]
\[ J_{j,C} = \tilde{J}_{j,C} \]

Term I, III, V still remain unclosed, and can be classified as 1) terms related to Reynolds stress tensor ($\sigma_{ij}$, subgrid stress tensor) and 2) related to subgrid scalar fluxes ($\tilde{u}_j''\phi''$). In addition, filtered flamelet parameters such as 3) subgrid variance of scalar ($\tilde{\phi}''^2$) and 4) subgrid scalar dissipation rate ($\tilde{\chi}$) are also needed to close the system of LES with flamelet combustion model. These four types of unclosed terms are closed with adaptive subgrid models and details of used models are described in the following Section.

3.3 Subgrid Modeling

3.3.1 The subgrid stress tensor, $\sigma_{ij}$

To close the unclosed term I shown in the filtered conservation momentum equation (Eq. (3.15)), the subgrid (residual) stress tensor $\sigma_{ij}$ have to be got by adaptive subgrid model. First of all, the subgrid stress tensor can be express as

\[ \sigma_{ij} = -\bar{\rho}u''_i u''_j \]
\[ = -\bar{\rho}(\tilde{\bar{u}}_i\tilde{\bar{u}}_j - \bar{u}_i\bar{u}_j) \]  

(3.21)
Smagorinsky model

The most commonly used subgrid model for the unclosed residual stress term was developed by Smagorinsky [21] based on an eddy viscosity assumption. With the eddy viscosity assumption, energy of the smallest scale eddy is in equilibrium, which means energy production and energy consumption rate is equal. By the Smagorinsky subgrid model, we can get expression of $\sigma_{ij}$ as

$$\sigma_{ij} - \frac{1}{3} \delta_{ij} \sigma_{kk} = 2\mu_t(\tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{kk}), \quad (3.22)$$

and the eddy viscosity

$$\mu_t = \bar{\rho}(C_S \Delta)^2 |\tilde{S}| \quad (3.23)$$

where $C_S$ is the Smagorinsky constant, and $|\tilde{S}| = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$. The smagorinsky constant $C_S$ is chosen in the range from 0.1 to 0.23 depending on the flow and grid resolution [22].

Dynamic Smagorinsky model

Germano [22] made a breakthrough in subgrid scale model by introducing dynamic model. In dynamic model, test filter $\hat{\Delta}$ (multiple of grid filter $\Delta$) is used and the model coefficient is calculated dynamically [16]. Lilly’s modification [23] is commonly used which uses a least squares technique to minimize the difference between the closure assumption and the resolved stresses.

3.3.2 The subgrid scalar fluxes, $\widetilde{u''_j}\phi''$

The subgrid scalar fluxes can be expressed as

$$\widetilde{u''_j}\phi'' = \widetilde{u_j}\phi - \widetilde{u_j}\bar{\phi} \quad (3.24)$$
In general, the gradient transport assumption is adapted for the modelling of subgrid scalar fluxes,

\[
\frac{u''_j}{\phi''} = -\zeta_t \frac{\partial \phi}{\partial x_j}
\]  

(3.25)

where \( \zeta_t \) is an eddy-diffusivity. Eddy-diffusivity is usually determined by eddy-viscosity \( (\mu_t) \) and non-dimensional numbers of turbulent reactive flow such as turbulent Prandtl number, \( Pr_t \), and turbulent Schmidt number, \( Sc_t \). For example,

\[
\zeta_t = \frac{\mu_t}{Pr_t}
\]  

(3.26)

3.3.3 The subgrid variance of scalar, \( \phi^{\prime\prime2} \)

For combustion simulation with LES, a reliable subgrid model for scalar fields is of particular importance [16]. With an assumption that the production and dissipation of variance is equal, Pierce and Moin [24] suggested the subgrid-scale Favre variance of scalar \( \phi^{\prime\prime2} \) as

\[
\phi^{\prime\prime2} = C \Delta^2 |\nabla \phi|^2
\]  

(3.27)

With the algebraical range of

\[
0 < \phi^{\prime\prime2} < 0.25
\]  

(3.28)

Coefficient C has to be selected adaptively by case and resolution of simulation. For example, if grid-filter size (\( \Delta \)) is small, the filtered variance value can be underestimated and bigger coefficient value is selected.

3.3.4 The subgrid scalar dissipation rate, \( \chi \)

For the subgrid scalar dissipation rate modelling, various algebraic equations can be used. Ihme [19] derived a model for the subgrid scalar dissipation rate as
\[
\tilde{\chi} = \frac{C_\chi C_\varepsilon \alpha_l}{Sc_t C_u} \tilde{\chi} \]

(3.29)

where, \(Sc_t = 0.4\), the coefficients \(C_\chi = 2\), and \(C_\varepsilon/C_u = 2\) are applied.

Domingo [25] used subgrid scalar dissipation model as below, with assuming a linear relaxation of the variance within the subgrid,

\[
\tilde{\rho} \tilde{\chi} = \bar{\rho} D |\nabla Z|^2 = \bar{\rho} D |\nabla \tilde{Z}|^2 + \bar{s}_\chi
\]

(3.30)

where,

\[
\bar{s}_\chi = \tilde{\rho} \frac{\tilde{Z}''^2}{\Delta^2/\nu_t}
\]

(3.31)

### 3.4 The system of governing equations for LES with flamelet approach

With derived filtered governing equations, subgrid models for complete closing, and adaptive assumption written above, complete system of governing equations for LES with flamelet approach is achieved as below.

1) continuity :

\[
\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j)}{\partial x_j} = 0
\]

(3.32)

2) momentum :

\[
\frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_i \tilde{u}_j + \delta_{ij} \tilde{\rho})}{\partial x_j} = \bar{p} g_i + \frac{\partial}{\partial x_j} [(\tilde{\rho} \alpha + \mu_t) (\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i})]
\]

(3.33)

3) scalar transport equation for mixture fraction :

\[
\frac{\partial (\tilde{\rho} \tilde{Z})}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j \tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} [(\tilde{\rho} \alpha + \frac{\mu_t}{Pr_t}) \frac{\partial \tilde{Z}}{\partial x_j}]
\]

(3.34)

4) subgrid variance of mixture fraction :

\[
\tilde{Z}''^2 = C \Delta^2 |\nabla \tilde{Z}|^2
\]

(3.35)
5-a) subgrid scalar dissipation rate (for SLFM):

\[ \bar{\chi} = \frac{C_\chi C_e}{S_C u} \frac{\alpha_1}{\Delta^2} \bar{Z}'' \]  

(3.36)

5-b) scalar transport equation for progress variable (for FPVA):

\[ \frac{\partial(\bar{p}\bar{C})}{\partial t} + \frac{\partial(\bar{p}\bar{u}_j\bar{C})}{\partial x_j} = \frac{\partial}{\partial x_j}[(\bar{p}\bar{\alpha} + \frac{\mu_t}{P_{rt}}) \frac{\partial\bar{C}}{\partial x_j}] + \bar{p}\bar{S}_C \]  

(3.37)

where \( \bar{\mu} = \mu(\bar{T}) \), \( \bar{\alpha} = \alpha(\bar{T}) \), and \( \bar{R} = R(\bar{Y}_\alpha) \). \( \bar{T}, \bar{Y}_\alpha, \bar{S}_C, \) and \( \bar{p}_{1D} \) are determined as a function of flamelet parameters, and finally all the chemical reaction related terms (\( \bar{\mu}, \bar{\alpha}, \bar{R}, \bar{T}, \bar{Y}_\alpha, \bar{S}_C, \) and \( \bar{p}_{1D} \)) are tabulated on a flamelet library. \( \bar{p}_{1D} \) is a density quantity at one-dimensional flamelet pressure condition (usually set as combustion chamber pressure in this study) and satisfies filtered EOS of ideal gas.

\[ \bar{p}_{1D} = \bar{p}_{1D} \bar{R} \bar{T} \]

With assumption that influence of pressure difference on turbulent combustion state can be ignore (means \( \bar{R} \) and \( \bar{T} \) is not changing by pressure achieved by turbulent solver), \( \bar{p} \) can be calculated as

6) EOS:

\[ \bar{p} = \frac{\bar{p}}{\bar{R}\bar{T}} = \frac{\bar{p}}{\bar{p}_{1D}} \bar{p}_{1D} \]  

(3.38)

Then, the system of governing equations of LES with flamelet model is closed perfectly, 8 unknown filtered values (\( \bar{p}, \bar{p}, \bar{u}_i, \bar{Z}, \bar{Z}'', \bar{\chi} \) or \( \bar{C} \)) with 8 equations (Eqs. (3.32) - (3.38)).
In this chapter, details of developed codes are described and categorized into two parts. First part is a describing of processes needed to generate flamelet libraries, consists of the calculation of one-dimensional laminar flamelet solution and the pdf integration. Second part is a describing of solver to solve entire system of governing equations for LES with flamelet combustion models. The developments of codes are all based on open-source modules (Cantera, Ember, OpenFOAM) and short introduction of these modules are also included.

4.1 Flamelet Library Generation

In flamelet combustion model, entire detail chemistry is acquired by a flamelet library. All filtered chemical variables, such as dynamic viscosity ($\mu$), thermal diffusivity ($\alpha$), mixture gas constant ($R$), temperature ($T$), species mass fraction ($Y_{\alpha}$), chemical source term of progress variable ($S_C$), density on laminar flamelet pressure condition ($p_{1D}$) of each state, are stored in a flamelet library.
as a function of flamelet parameters \((\bar{Z}, Z'^2, \bar{\chi})\) or \((\bar{Z}, Z'^2, \bar{C})\). The first step of generating flamelet library is calculating the one-dimensional laminar flamelet which ensembles turbulent flamelet. In this study, two methods to calculate one-dimensional laminar flamelet based on open-source modules are developed. One is method with ‘Cantera module’ which can calculate steady flamelet solutions on the steady burning brach of S-curve (Figure 2.3). The other is method with ‘Ember module’ which can calculate transient flamelet solutions varying strain rates conditions. The second step for the flamelet library generation is a PDF integration step. With PDF integration, turbulence-combustion interactions are implied on flamelet solutions. Detail procedures of each step are described below.

4.1.1 One-dimensional laminar flamelet calculation with Cantera module

Steady flamelet calculation solver with Cantera module

Cantera [26] is a chemical kinetics, thermodynamics, and transport tool suite which can be used for chemical reaction calculations as shown in Figure 4.1.

![Figure 4.1 Schematic algorithm of cantera module](image)

Figure 4.1 Schematic algorithm of cantera module
Using Cantera, laminar counter-flow diffusion flames (the schematic configuration are shown in Figure 4.2) are solved by Newton-Rhapson methods at each strain rate by setting inlet velocities accordingly keeping the physical domain size constant.

**Transformed to mixture fraction \( (Z) \) domain**

Using Cantera module, chemical quantities are calculated on physical domain. (i.e. calculated temperature solutions on physical domain is shown in Figure 4.3) The flamelet solutions on the physical space have to be transformed to the mixture fraction space according to specific definitions of mixture fraction as mentioned on Chapter 2. In this study, Barlow’s definition (Eq. (2.3)) is used.

**Validation of transformed steady flamelet solutions**

To validate the solutions achieved with developed solver, transformed solutions are compared with FlameMaster solutions. FlameMaster is a C++ computer
Figure 4.3 Temperature solution of a laminar flamelet on physical domain and on mixture fraction domain, $\chi_{st}=1 \ s^{-1}$

program for zero-D combustion and one-D laminar flame calculations, including solvers for potential flow laminar flames in mixture fraction domain. As seen in Figure 4.4, some of achieved chemical quantities, temperature and mass fraction of species, calculated by the developed solver using Cantera module shows good agreement with the solutions obtained using FlameMaster.

**Procedures and tips for calculating a group of steady flamelets**

When starting a calculation for a condition, we have two options for the initial solution. One is setting initial solution using equilibrium calculation of the condition, and the other is using previous case’s solutions for the initial condition of the current case. Refer to our experience, start calculation with the smallest inlet velocity, almost zero scalar dissipation rate, which uses equilibrium calculation as initial guess and increasing inlet velocity conditions is good to get entire steady flamelet solutions. When increasing inlet velocity conditions and restart calculation, the solutions of previous condition are used as initial solutions. With this procedure, we can get the most smooth and stable solutions for a flamelet library as shown in Figure 4.5. As shown in S-curve, as stoichio-
Figure 4.4 Validation of transformed laminar flamelet solutions \((T, Y_{H2O}, Y_{CO2})\) with flameMaster solutions, \(\chi_{st} = 1 \text{ s}^{-1}\)
metric scalar dissipation rate is increasing, maximum temperature of a flamelet is decreasing and eventually extinguished.

Figure 4.5 Entire steady flamelet solutions (e.g. Temperature) achieved by developed solver and plot of stochiometric scalar dissipation rate ($\chi_{st}$) versus maximum temperature ($T_{max}$) of flamelet solutions, S-curve

### 4.1.2 One-dimensional laminar flame calculation with Ember module

**Transient flamelet calculation solver with Ember module**

To get transient solutions on the unstable branch of S-curve (Figure 2.3), a flamelet calculation solver using Ember is developed. Ember [27] is a quasi-one-dimensional, unsteady reacting flow module, which can be used to simulate a number of fundamental flame configurations. In this study, unsteady laminar equations of potential flow are solved in transient manner varying strain rates. Solutions in physical domain need to be transformed on mixture fraction domain. Transform function to mixture fraction space also implemented in code as same as in the code for steady-flamelet calculation.
Procedures and tips for calculating a group of transient flamelets

First, we have to find the strain rate that extinction started, as increasing strain rate conditions. At the critical point, with a little change of strain rate, flamelet solutions go to extinction solutions. Maintaining the critical strain rate condition, the solution just before the critical strain rate is used for initial solution of calculation. Then, transient unstable solutions during the extinction process is achieved as black line in Figure 4.6. Transient solutions are stored about 20 K of difference of maximum temperature of each solutions. If transient solutions are too coarse, interpolation of values (typically, chemical source terms $\tilde{w}_C$ which has stiff change on mixture fraction and progress variable domain) shows a poor performance. When getting maximum temperature of each flamelet as a function of scalar dissipation rate, we can remind the transient solutions are on same scalar dissipation rate (Figure 4.6). In order to include these transient flamelets on flamelet library, implementation of extension process to progress variable (C) space is required.

Figure 4.6 Entire flamelet solutions (e.g. Temperature) achieved by developed solver (black : transient solutions, gray : steady solutions) and plot of stori- chiometric scalar dissipation rate ($\chi_{st}$) versus maximum temperature ($T_{max}$) of entire flamelet solutions, S-curve
Extension to progress variable domain

To extend flamelet library of SLFM to FPVA which include transient solutions, flamelet solutions have to extend to progress variable domain. As demonstrate on chapter 2.3, various progress variable definition (Eqs. (2.6), (2.7), (2.8)) can be implemented. With the definition of

\[ C = \frac{Y_{H2}}{M_{H2}} + \frac{Y_{H2O}}{M_{H2O}} + \frac{Y_{CO2}}{M_{CO2}} \]

flamelet solutions on mixture fraction space (as shown in Figure 4.6) can be extended to mixture fraction\((Z)\) and progress variable\((C)\) domain as Figure 4.7.

Figure 4.7 Entire solutions extended on the progress variable domain
4.1.3 PDF integration

To consider the turbulence-combustion interaction on subgrid scale, integration step with probability distribution function (PDF) is applied on flamelet solutions. With PDF integration, Favre-filtered scalar chemical quantities $\bar{\phi}$ ($\bar{T}$, $\bar{Y}_\alpha$, $\bar{S}_C$) and filtered density $\bar{\rho}$ are calculated as,

filtered scalar chemical quantities, $\bar{\phi}$:

$$\bar{\phi} = \int_{\psi_{1,\text{min}}}^{\psi_{1,\text{max}}} \ldots \int_{\psi_{n,\text{min}}}^{\psi_{n,\text{max}}} \phi(\psi_1, \ldots, \psi_n) \bar{P}(\psi_1, \ldots, \psi_n) d\psi_n, \ldots, d\psi_1 \quad (4.1)$$

filtered density, $\bar{\rho}$:

$$\bar{\rho}^{-1} = \frac{1}{\bar{\rho}} = \int_{\psi_{1,\text{min}}}^{\psi_{1,\text{max}}} \ldots \int_{\psi_{n,\text{min}}}^{\psi_{n,\text{max}}} \rho^{-1} \bar{P}(\psi_1, \ldots, \psi_n) d\psi_n, \ldots, d\psi_1$$

$$\bar{\rho} = \left[ \int_{\psi_{1,\text{min}}}^{\psi_{1,\text{max}}} \ldots \int_{\psi_{n,\text{min}}}^{\psi_{n,\text{max}}} \rho^{-1} \bar{P}(\psi_1, \ldots, \psi_n) d\psi_n, \ldots, d\psi_1 \right]^{-1} \quad (4.2)$$

where $\psi$ represents parameters of flamelet solutions. The parameters are chosen as mixture fraction ($Z$) and scalar dissipation rate ($\chi$) with SLFM, otherwise, mixture fraction ($Z$) and progress variable ($C$) with FPVA. For both combustion model (SLFM, FPVA), same detail PDF integration procedure is used in this study, except for ($\chi$) is substituted by ($C$). Therefore, detail procedures below are explained only in a point of view FPVA.

By Eqs. (4.1) and (4.2), PDF integration equations for filtered values with FPVA combustion model become

$$\bar{\phi} = \int_{Z_{\text{min}}}^{Z_{\text{max}}} \int_{C_{\text{min}}}^{C_{\text{max}}} \phi(Z, C) \bar{P}(Z, C) dC dZ \quad (4.3)$$

$$\bar{\rho} = \left[ \int_{Z_{\text{min}}}^{Z_{\text{max}}} \int_{C_{\text{min}}}^{C_{\text{max}}} \rho^{-1}(Z, C) \bar{P}(Z, C) dC dZ \right]^{-1} \quad (4.4)$$

where the joint probability,

$$\bar{P}(Z, C) = \bar{P}(C|Z) \bar{P}(Z) \quad (4.5)$$
Statical distributions of flamelet library parameter ($\tilde{P}(Z)$, $\tilde{P}(C|Z)$) are calculated or achieved by function of subgrid scalar fluctuations. For the conserved scalar ($Z$), presumed $\beta$-PDF is normally used [16]. Presumed $\beta$-PDF is an algebraic function that is determined by filtered scalar ($\tilde{\phi}$) and subgrid-scale Favre variance ($\tilde{\phi}^{n2}$). For mixture fraction, the presumed $\beta$-PDF follows

$$\tilde{P}(Z) = Z^{\alpha-1}(1-Z)^{\beta-1}\frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}$$  \hspace{1cm} (4.6)$$

$$\alpha = \tilde{Z}(\frac{\tilde{Z}(1 - \tilde{Z})}{Z^{n2}} - 1)$$  \hspace{1cm} (4.7)$$

$$\beta = (1 - \tilde{Z})(\frac{\tilde{Z}(1 - \tilde{Z})}{Z^{n2}} - 1)$$

For the reactive scalar ($C$), delta function, which ignore subgrid variance effect, is used and written as

$$\tilde{P}(C|Z) = \delta(C - \tilde{C}|Z)$$  \hspace{1cm} (4.8)$$

where $\lambda$ satisfies

$$\tilde{C} = \int C(Z, \lambda_0)\tilde{P}(Z)dZ$$  \hspace{1cm} (4.9)$$

$\lambda$ (or $\psi$) represents a flamelet parameter which is used for parameterization of the family of flamelet solutions, such as temperature at stoichiometric mixture fraction ($T_{st}$), maximum progress variable value of each flamelet solution ($C_{p,max}$). After PDF integration of flamelet solutions, filtered chemical variables are matched with function of filtered parameters ($\tilde{Z}$, $\tilde{\phi}^{n2}$,  $\tilde{C}$). Using ‘griddata’ function of matlab, interpolation is conducted between flamelet solutions. Finally, Flamelet library is generated and stored on three-dimension as shown in Figure 4.8 and 4.9.
Figure 4.8 Flamelet library solutions ($\tilde{T}$), when $\tilde{Z}^{\nu 2} = 0$ and 0.25
Figure 4.9 Flamlet library solutions ($\tilde{S}_C$), when $\tilde{Z}^{r2} = 0$ and 0.25
4.2 Solver Algorithm

4.2.1 Open-source field operation and manipulation (OpenFOAM)

LES solver with flamelet approach is developed based on OpenFOAM toolbox. OpenFOAM is a toolbox which was originally developed as a high-end $C++$ classes library (Field Operation and Manipulation) [28]. The OpenFOAM toolbox is opensource tools which can be developed and modified freely by large user groups. As many users use the tools, the speed of developing is accelerated. Today, the OpenFOAM supports various tools for numerical simulation of complex fluid flows involving chemical reactions, turbulence and heat transfer, to acoustics, solid mechanics and electro-magnetics. Based on ‘rhoreactingFoam’ which is a basic solver included in OpenFOAM toolbox, modifications for the flamelet combustion model is implemented.

4.2.2 Code organization

Procedure of new implementation for flamelet approach is presented in Figure 4.10. The conventional ‘rhoreactingFoam’ is modified to solve additional governing equations derived by previous chapter and to get thermodynamic properties, density, and the chemical source term of progress variable by flamelet library prepared in advance. Pressure-velocity coupling of continuity and momentum equation is solved using merged PISO-SIMPLE (PIMPLE) algorithm.
Velocity pressure coupling: PIMPLE algorithm

Continuity:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

Momentum:
\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + 2\nabla \cdot ((\mu + \mu_t) \mathbf{S}) \]

Mixture fraction scalar transport equation:
\[ \frac{\partial (\rho \tilde{Z})}{\partial t} + \frac{\partial (\rho \tilde{u}_j \tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \rho \tilde{u}_i + \frac{\mu_t}{P_{rt}} \right) \frac{\partial \tilde{Z}}{\partial x_j} \right] \]

Mixture fraction variance algebraic equation:
\[ \tilde{Z} n^2 = C \Delta^2 \nabla \tilde{Z}^2 \]

Subgrid scalar dissipation rate:
\[ \tilde{\chi} = \frac{C_x C_c}{S_c C_u} \alpha \Delta^2 \tilde{Z} n^2 \]

Progress Variable scalar transport equation:
\[ \frac{\partial (\rho \tilde{C})}{\partial t} + \frac{\partial (\rho \tilde{u}_j \tilde{C})}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\rho \tilde{u}_i + \frac{\mu_t}{P_{rt}}) \frac{\partial \tilde{C}}{\partial x_j} \right] + \rho \tilde{S}_C \]

Figure 4.10 Procedure of new implementation on OpenFOAM module
In this chapter, validation for our new developed codes is conducted. Partially premixed jet flame, Sandia flame D, is chosen as a validation case. Details of simulation and the simulation results compared with experiment data of Sadia flame D is suggested.

5.1 Background

To validate our new solver, partially premixed jet flame (Sandia flame D) is chosen as a validation case. The experiment of Sandia flame D was conducted by Barlow and Frank [29] and well-documented information is available as part of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF workshop) [30]. Due to the well defined experi-
mental conditions and the availability of detailed data, it has become one of the canonical turbulent flames used frequently for the purpose of validation of computational modeling and simulations.

Sandia flame D is a partially premixed $CH_4$/air flame assisted by a pilot flame. Partially premixed component with 75 percent of methane and 25 percent of air by volume is used for fuel and air is used for oxidizer. Reynolds number of the flame is calculated as 22400 and stoichiometric mixture fraction $Z_{st}$ is 0.351 with a small degree of local extinction [29]. Table 5.1 shows details of the experimental condition.

Figure 5.1 Piloted $CH_4$/Air Flame D
Table 5.1 Experiment inlet conditions of Sandia D flame

<table>
<thead>
<tr>
<th></th>
<th>Fuel</th>
<th>Pilot</th>
<th>Coflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>U [m/s]</td>
<td>49.6</td>
<td>11.4</td>
<td>0.9</td>
</tr>
<tr>
<td>T [K]</td>
<td>294</td>
<td>1880</td>
<td>291</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
<td>0.271</td>
<td>0</td>
</tr>
</tbody>
</table>

5.2 Case Details

Flamelet library generation

Flamelet library with experiment conditions of sandia flame D is generated. One-dimensional laminar flamelet solutions are calculated using developed codes with Cantera and Ember module as explained above. The detailed GRI-Mech 3.0 chemical mechanism is used with 53 species and 325 reaction steps, which is an optimized mechanism designed to model natural gas combustion including NO formation and reburn chemistry [31]. For the mixture fraction ($Z$), Barlow’s definition (Eq (2.3)) is used, which is repeated here:

$$ Z = \frac{Z_C/(mW_C) + Z_H/(nW_H)}{Z_{C,1}/(mW_C) + Z_{H,1}/(nW_H)} $$

For the progress variable ($C$), sum of mass fractions of $H_2$, $H_2O$, $CO_2$ divided by molecular weight is used.

$$ C = \frac{Y_{H_2}/M_{H_2} + Y_{H_2O}/M_{H_2O} + Y_{CO_2}/M_{CO_2}}{Z_{\overline{Z}, \overline{Z^2}}} $$

For SLFM flamelet library, which use ($\overline{Z}$, $\overline{Z^2}$, $\overline{\chi}$) as flamelet parameters, total 101 mixture fraction ($\overline{Z}$) is used from 0 to 1, stepping 0.01. total 26 mixture fraction variance ($\overline{Z^2}$) value is used from 0 to 0.25 stepping 0.01.
For $\tilde{\chi}$, as same number as solved laminar flamelets, total 29 scalar dissipation rate ($\chi$) is used. For FPVA flamelet library, which use $(\tilde{Z}, \tilde{Z}^2, \tilde{C})$ as flamelet parameters, total 101 normalized progress variable ($\tilde{C}$) is used instead of scalar dissipation rate ($\chi$) from 0 to 1, stepping 0.01.

**Computational domain and mesh**

Computational domain size is $80D_{Fuel}$ for axial direction and $26.5D_{Fuel}$ for radial direction. Grids are clustered to center of domain and near nozzles, to resolve the region of interest. An anatomy of the total computational domain are shown as Figure 5.2. In full three-dimensional cases for large eddy simulations (LES), 3.4 million cells were used. Figure 5.3 shows clustered mesh in a cross-section and mesh size normalized by diameter of fuel nozzle ($D_{Fuel}$) as a function of radial location.

![Figure 5.2 Computational domain and zoom in the center](image-url)
Numerical discretization

For solving the system of governing equations, the standard finite volume method is employed. Constant courant number 0.4 is set during calculations. For the temporal discretization, the explicit Euler method is used. For the convective terms of scalar transport equations, Van Leer’s third-order accurate MUSCL scheme is used, while filteredLinear2V scheme, which is a modified linear scheme to remove high-frequency modes with ‘staggering’, is used for the convective terms in the momentum equations.

5.3 Apriori Study on Flamelet Library

Previous to perform LES for the Sandia flame D, an a priori study to validate flamelet library is performed. Accuracy of LES for turbulent combustion is influenced by various components of modeling, such as subgrid models, numerical schemes, and combustion model used. In the simulation with flamelet model, flamelet libraries represent all the combustion effect and the validation of flamelet library is important in perspect of discretely attributing the errors.
to the library or to the other numerical factors.

Based on well-documented measurements of Sandia flame D, flamelet databases previous to filtered stage can be compared with the instantaneous scatter data. With the flame D, instantaneous scatter data at several downstream stations and mean and variance data during several flow times were achieved for temperature, species mass fractions, and mixture fraction.

Figure 5.4 shows flamelet library solutions of temperature and major species mass fraction of \( H_2O, H_2, CO_2, CO, NO \) compared with scatter data of sandia flame D. Scatter data is classified by colors as the location along downstream. Yellow is measurements at 0.075\( D_{Fuel} \), cyan is measurements at 15\( D_{Fuel} \), purple is measurements at 30\( D_{Fuel} \), green is measurements at 45\( D_{Fuel} \), blue is measurements at 60\( D_{Fuel} \), gray is measurement at 75\( D_{Fuel} \). Measurements from 0.75\( D_{Fuel} \) and 15\( D_{Fuel} \), where strain rate is high because of inlet flows, exist near the critical flamelet solution. Measurements at 30\( D_{Fuel} \), where maximum flame temperature is located, exist near 0 strain rate flamelet solution. Because flame D case is a stable flame with a small degree of extinction, majority of the states in the flame D exists between near 0 strain rate flamelet solution and extinction flamelet solution. Majority of flame measurements are well contained by achieved flamelet solutions, except for \( NO \). In case of \( NO \), the mass fraction of \( NO \) is over-predicted by flamelet solutions. It seems the inconsistency of reaction time scale is the major cause of over-prediction. Time scale is a critical factor in \( NO \) generation process. However, with steady flamelet solution, the influence of reaction time scale cannot be included correctly. It can be thought the limitation of steady flamelet combustion model.
Figure 5.4 Flamelet library solutions compared with scatter data of sandia flame D (yellow : location at $0.075D_{Fuel}$, cyan : location at $15D_{Fuel}$, purple : location at $30D_{Fuel}$, green : location at $45D_{Fuel}$, blue : location at $60D_{Fuel}$, gray : location at $75D_{Fuel}$)
5.4 Simulation Results

With steady laminar flamelet model

Figure 5.5 shows axial profile of temperature and mixture fraction along downstream. Instantaneous (dotted line) and mean (solid line) values are shown with experiment measurements (symbol). Mean values are calculated by averaging during 5 - 6 times of flow time while instantaneous value is got from a moment. Figure 5.6 shows radial profile of temperature and mixture fraction at $x/D_{Fuel} = 4, 15, 45$. Black lines and symbol denote temperature results, while blue lines and symbol denote mixture fraction results. Temperature and mixture fraction results with SLFM are in a reasonable agreement with experimental data of sandia flame D. Mixture fraction is a principle parameter in flamelet models and determines the location of flamelet. Therefore, the reasonable agreement of mixture fraction means reasonable chemical reaction terms are achieved by adaptable flamelet library. The agreement of temperature results also validates the chemical reaction of the flame is reasonably calculated by developed solver with SLFM. Instantaneous temperature contour of LES with SLFM model is shown in Figure 5.7.

Figure 5.5 Axial profile of temperature and mixture fraction along downstream
Figure 5.6 Radial profile of temperature and mixture fraction at $x/D_{fuel} = 4, 15, 45$

Figure 5.7 Instantaneous temperature contour of LES results with SLFM
With flamelet progress variable model

Figure 5.8 shows axial profile of temperature and mixture fraction along downstream. Same with SLFM results above, instantaneous (dotted line) and mean (solid line) values are shown with experiment measurements (symbol). Mean values are calculated by averaging during 5 - 6 times of flow time while instantaneous value is got from a moment. Figure 5.9 shows radial profile of temperature and mixture fraction at $x/D_{Fuel} = 4, 15, 45$. Black lines and symbol denote temperature results, while blue lines and symbol denote mixture fraction results. Temperature and mixture fraction results with FPVA are also in a reasonable agreement with experimental data of sandia flame D. Instantaneous temperature contour of LES with FPVA model is shown in Figure 5.10.

![Figure 5.8 Axial profile of temperature and mixture fraction along downstream](image)

Compared SLFM and FPVA results

Simulation with both flamelet combustion model, SLFM and FPVA, shows good agreement with experiment measurements. It seems that Sandia flame D is with a small degree of local extinction, both combustion model show similar performance whether unstable branch is include or not. However, it shows
Figure 5.9 Radial profile of temperature and mixture fraction at $x/D_{Fuel} = 4, 15, 45$

Figure 5.10 Instantaneous temperature contour of LES results with FPVA
noticeable difference on high strained region near nozzles as show in Figure 5.11.

![Figure 5.11 Zoom in temperature contour near the nozzle (left : SLFM, right : FPVA)](image)

Figure 5.11 Zoom in temperature contour near the nozzle (left : SLFM, right : FPVA)
6.1 Conclusions

In this study, codes for LES with flamelet combustion model are developed based on open-source modules (Cantera, Ember, and OpenFOAM). Flamelet libraries for two kinds of flamelet models, SLFM and FPVA, can be generated by codes developed using Cantera and Ember module. Open-source solver, ‘rhoReactingFoam’, of OpenFOAM module is modified to read chemical reaction quantities from flamelet library and to solve additional transport equations for flamelet parameters. Dynamic subgrid model is used to close subgrid terms, while algebraic subgrid model is used for modelling subgrid variance of mixture fraction $\overline{Z^{r2}}$ and subgrid scalar dissipation rate $\overline{\chi}$.

Validation for the developed codes has been conducted for the partially premixed methane-air flame, Sandia flame D. An apriori study for flamelet library conducted to validate flamelet library itself, shows good agreement with experiment data in that thermochemical state of turbulent flame is well repre-
sented by the flamelets. LES results with both flamelet model also show good agreement with the measurement.

6.2 Future Work

The present study is a foundation of future development for the modeling of turbulent combustion in LES. Here some directions for further development is suggested.

Further an apriori study for comparing transient flamelet solutions from ignition process and extinction process against the experimental data will prove the importance of introducing transient pathways into the flamelet library.

In the practical systems, the combustion process is not adiabatic because of the radiative and/or conductive heat loss to the surroundings. One may include the effect of heat loss by constructing flamelet libraries at different level of enthalpy and solve energy equation including sink terms and/or boundary conditions.
Bibliography


초록

난류 연소는 산업용 발전기, 디젤 엔진, 가스터빈 엔진, 로켓 등 실용적 연소기의 연소유동장에서 나타나는 핵심 현상으로, 고성능의 장치를 설계하기 위해서는 난류연소 현상 자체의 특성들에 대한 연구가 필수적으로 이루어져야한다. 특히 장치의 연소효율 (efficiency), 연소 안정성 (stability), 오염물질 배출도 (pollutant emission) 등은 난류연소에서 대두되는 핵심 주제로서 적절한 실험적, 수치적 연구가 필히 요구된다. 최근 large-eddy simulation (LES) 난류 수치기법, 동적 서브그리드 (dynamic subgrid) 모델의 개발과 함께 컴퓨터 계산 성능의 비약적인 발전이 이루어지면서 난류연소의 수치적 연구가 활발하게 이루어지고 있다. 특히, 플레임렛 연소모델을 적용한 LES 해석은 실물에서 일어나는 연소현상 연구를 위한 대표적인 방법으로서 많은 연구가 수행되고있다. 본 연구에서는 오픈소스 모듈에 기반한 플레임렛 연소모델 (SLFM, FPVA)을 적용한 LES 수치해석 코드를 개발하였다. 본 논문에는 사용된 플레임렛 연소모델과 LES 난류 모델에 대한 전반적인 이론 정리와 함께, 개발된 수치해석 코드와 이를 통한 수치해석 방법에 대한 체계적인 정리를 수행하였다. 실험데이터를 확보할 수 있는 모델화염으로 부분 혼합화염 (partially premixed flame)인 산디아 화염 D (Sandia flame D)를 선정하여 코드 검증을 위한 수치해석을 수행하였다.

주요어: LES, 플레임렛 연소모델, 난류연소, 비혼합화염, 수치해석
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