Development of a Large-Eddy Simulation Solver for Turbulent Combustion Using Flamelet Combustion Models

In aerospace applications, such as aircraft gas turbine engines, scramjet engines, and rocket engines, turbulent combustion is the primary method to generate energy. 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.

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. Large-eddy simulation (LES) with flamelet combustion model 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.

The purpose of the present study is two-fold: one is to obtain an overview of theories and derivations for LES with flamelet combustion model. The other is to develop an LES solver with flamelet combustion model, which has capacity to simulate turbulent combustion with higher accuracy and lower computational cost.

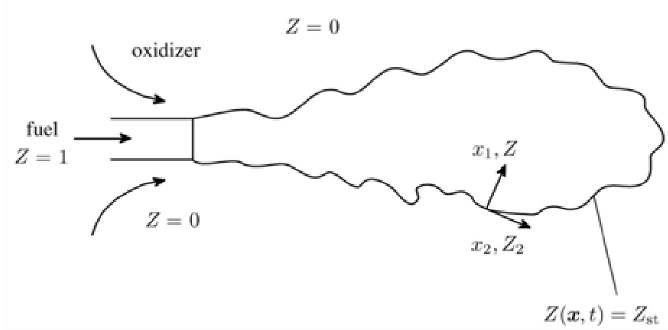

Figure 1. Concept of flamelet combustion model

First, details of flamelet combustion models and related theories are introduced. 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 appoach (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 (χ), and progress variable (C) are described together.

Next, the system of governing equations of LES with flamelet model is described. 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. The final closed system of filtered governing equations for LES with flamelet combustion model can be written as below.

1) continuity :

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j}{\partial x_j} = 0$$

2) momentum :

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \delta_{ij}\overline{p})}{\partial x_j} = \overline{\rho}g_i + \frac{\partial}{\partial x_j}[(\check{\mu} + \mu_t)(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i})]$$

3) scalar transport equation for mixture fraction :

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

4) subgrid variance of mixture fraction :

$$\widetilde{Z''^2} = C\Delta^2|\nabla\widetilde{Z}|^2$$

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

$$\widetilde{\chi} = \frac{C_\chi C_\epsilon}{Sc_t C_u}\frac{\alpha_t}{\Delta^2}\widetilde{Z''^2}$$

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

$$\frac{\partial (\overline{\rho}\widetilde{C})}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{u}_j\widetilde{C})}{\partial x_j} = \frac{\partial}{\partial x_j}[(\overline{\rho}\check{\alpha} + \frac{\mu_t}{Pr_t})\frac{\partial \widetilde{C}}{\partial x_j}] + \overline{\rho}\widetilde{S}_C$$

6) EOS :

$$p = \overline{\rho}\check{R}\widetilde{T}$$

Next, details of developed codes are described. The overall algorithms can be 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.

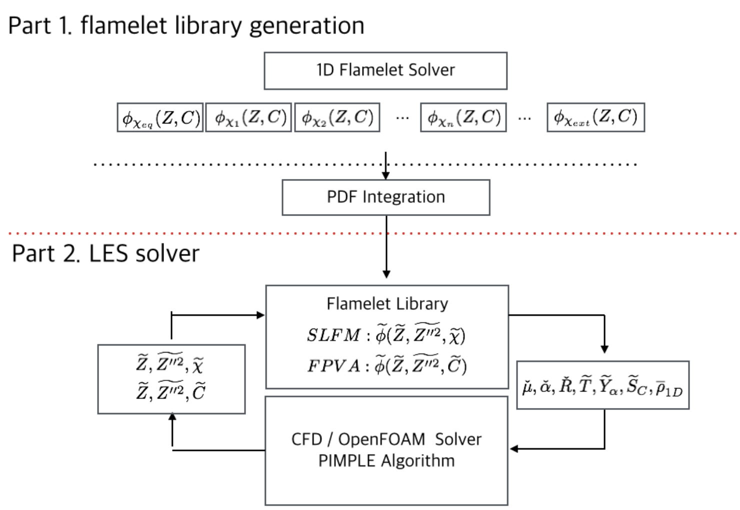

Figure 2. Algorithms of developed codes

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 (Figure 3), shows good agreement with experiment data in that thermochemical state of turbulent flame is well represented by the flamelets. Large-eddy simulation results of developed codes (Figure 4 and 5) also show good agreement with the measurement. Figure 6 shows instantaneous temperature contour of simulation results.

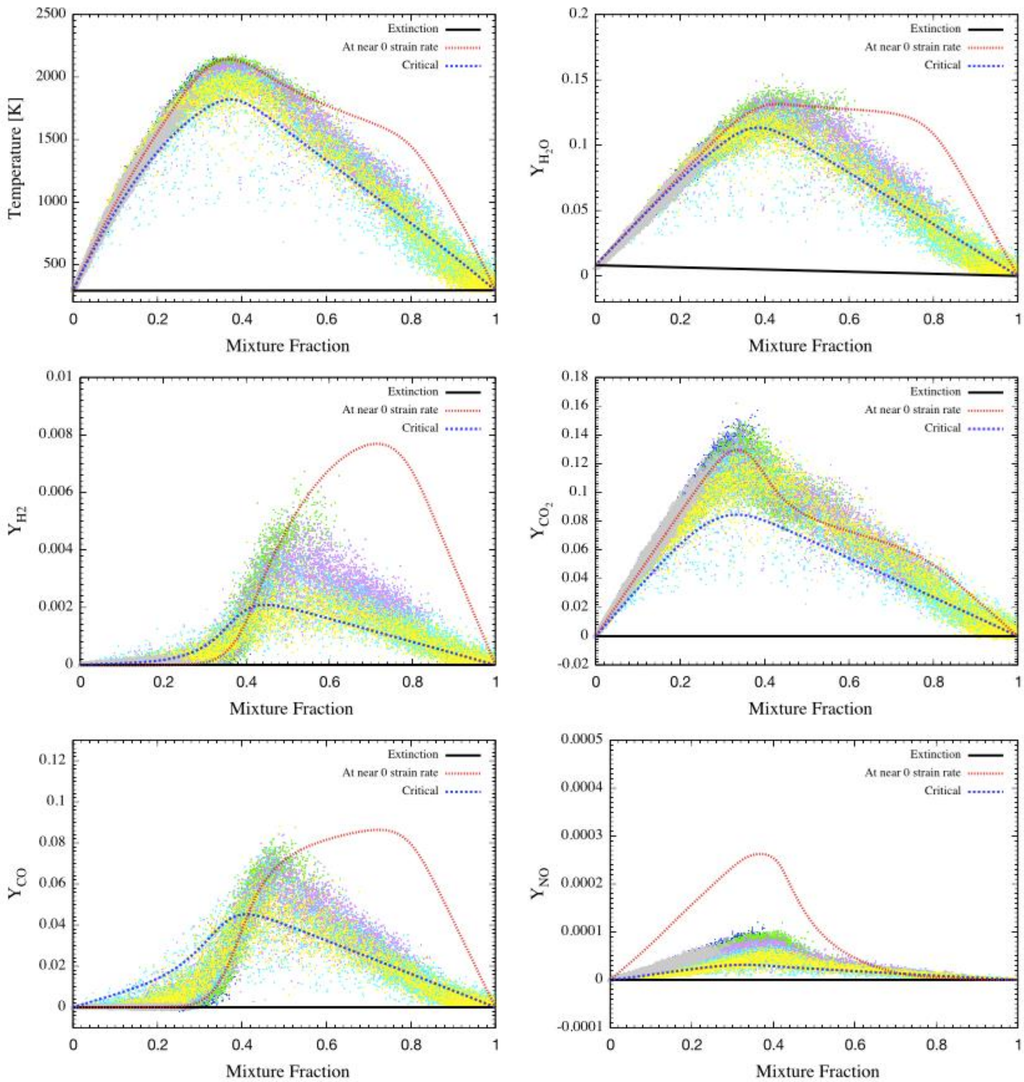

Figure 3. Flamelet library solutions compared with scatter data of Sandia flame D (yellow : location at 0.075D_Fuel, cyan : location at 15D_Fuel, purple : location at 30D_Fuel, green : location at 45D_Fuel, blue : location at 60D_Fuel, gray : location at 75D_Fuel)

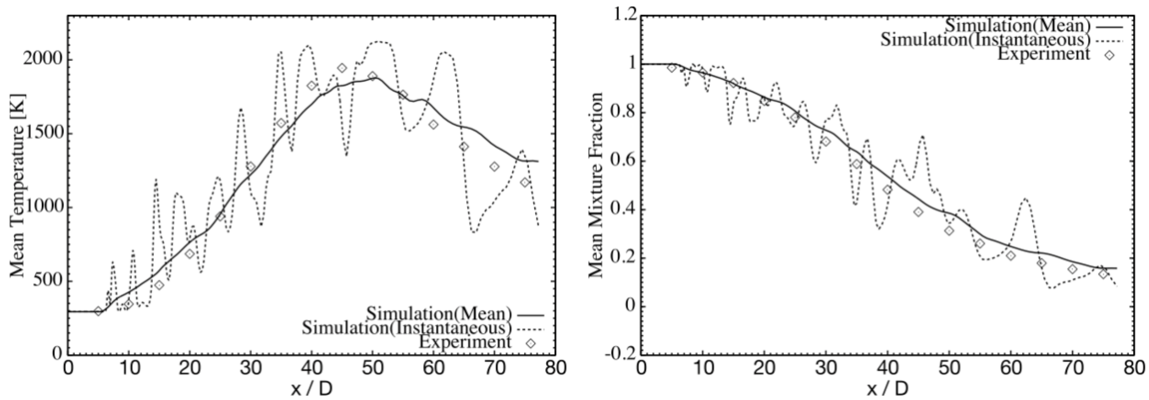

Figure 4. Axial profile of temperature and mixture fraction along downstream

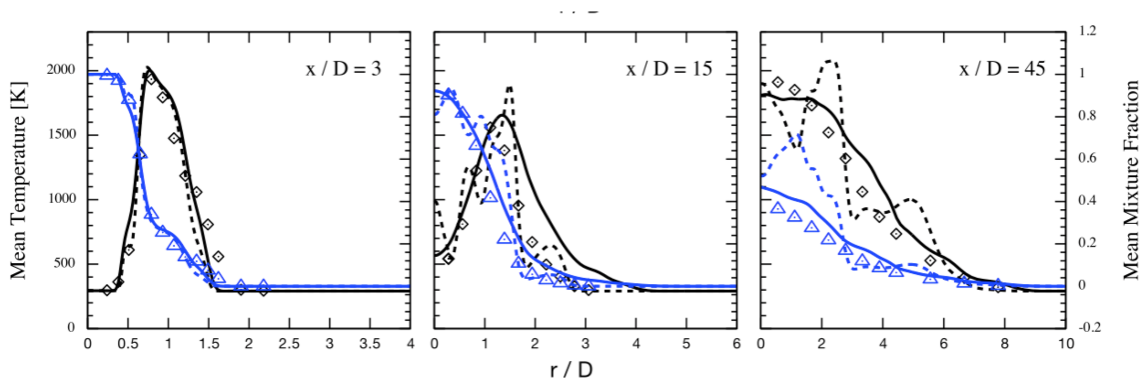

Figure 5. Radial profile of temperature and mixture fraction at x/D_Fuel = 4, 15, 45

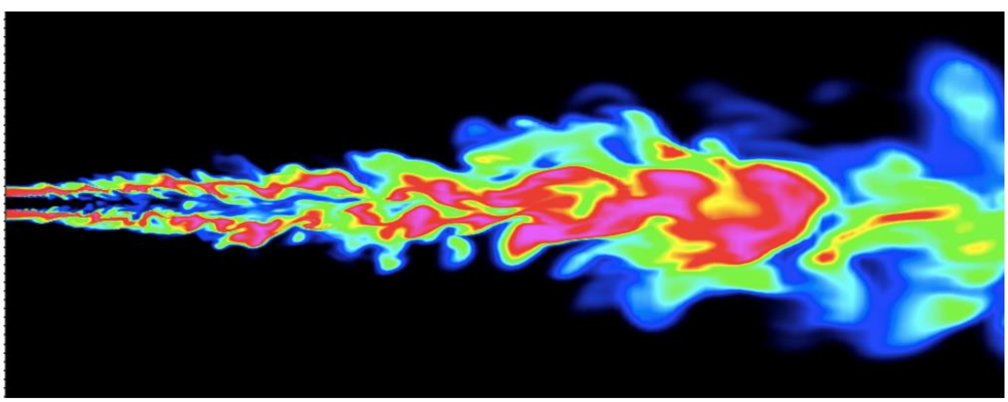

Figure 6. Instantaneous temperature contour of simulation results

The present study is a foundation of future development for the modeling of turbulent combustion in LES. Some directions for further development is suggested. With the future development, more accurate simulation and prediction of turbulent combustion phenomena will be made. With the developed solver, flame characteristics such as combustion efficiency, stability, and pollutant emissions of turbulent combustion can be achieved. These results can be applied for developing high performance engines of aerospace devices.