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A FGM/PDF SOLVER FOR SIMULATIONS OF TURBULENT REACTING FLOWS IN OPENFOAM

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ABSTRACT

*In this study, a new FGM/PDF [*Van Oijen, 2016*] solver is developed within OpenFOAM for the simulations of turbulent reacting flows. The turbulent-chemistry interaction is modeled by presumed β-PDF method. The chemical calculations are reduced using Flamelet Generated Manifold (FGM) method. One dimensional flamelets are generated from premixed flame calculations using Cantera. The solver has the capability of performing in both RANS and LES contexts. The performance of the new solver for the non-premixed, premixed and partially premixed turbulent flames on non-swirling and swirling conditions are evaluated using Sandia Flame D [Barlow et al. 1998] and Cambridge-Sandia Stratified flames [*Sweeney et al. 2012*]. The results demonstrate a good predictive capability of the new solver.*

INTRODUCTION

In all practical combustion devices, i.e., gas turbines in power plants, aircraft engines, the combustion takes place in a turbulent environment. Therefore, understanding of the fundamentals of the turbulent reacting flows is crucial to design an efficient, reliable and robust combustion device. However, since turbulent reacting flows involve very large range of time and length scales, their direct numerical prediction requires to resolve all time and length scales, which results in an infeasible computational cost. Additionally, since the chemical reaction mechanism involves hundreds of elementary reactions and chemical species, the detailed calculations of the chemistry requires significant amount of computational time.

To model the turbulent motions, various turbulent models have been introduced in the RANS and LES context to reduce the computational time. In the RANS context, the numerical solutions are seek for the mean flow fields by modelling turbulent fluctuations at all scales. In the LES context, the turbulent motions are split into large and small scales. Then the large scales are calculated explicitly by modelling the effects of the small scales.

The combustion chemistry takes place at the smallest length scale in a turbulent reacting flow, therefore the interaction between turbulence and chemistry have to be modelled in both the RANS and LES contexts. Various turbulent combustion models have been introduced in

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literature [Peters, 1984; Pierce and Moin, 2004; Pitsch et al. 1998; Pope, 1985]. In this study, the *presumed β-PDF* model is employed to model the turbulence-chemistry interaction.

Furthermore, to reduce computational cost of the detailed chemistry calculations, the reduction methods have been developed. The FGM method reduces the detailed chemistry calculation into a two-dimensional manifold parameterized by mixture fraction and progress variable [Van Oijen, 2016].

The aim of this study is to develop a robust FGM/PDF solver for the simulation of turbulent reacting flows in practical gas turbine devices. The solver is developed in OpenFOAM, an open-source platform of continuum mechanics. The predictive capability of the new solver is evaluated by non-premixed Sandia D flame [Barlow et al. 1998] as well as premixed and partially premixed turbulent flames on swirling and non-swirling conditions from Cambridge–Sandia stratified flame series [Sweeney et al. 2012].

METHOD

The FGM/PDF method developed in this study will be explained and presented in three section: i) the formulation in RANS and LES context, ii) the FGM chemical reduction method, iii) the modeling of turbulence-chemistry interaction: presumed *β*-PDF method.

The formulation of RANS and LES methods

The turbulent reacting flow is represented by the mean (or filtered) mass and momentum equations in RANS (or LES, respectively) context. The turbulent fluctuations are modelled using turbulent models. The low-Mach number assumption is employed, thus the density is decoupled from the pressure fields and calculated based on the chemical reactions. The thermochemical properties (i.e., temperature, density, and chemical species) are retrieved from a four-dimensional lookup-table parameterized by the mean and variance of mixture fraction and progress variable. Therefore, four additional transport equations for the mean and variance of mixture fraction and progress variable are solved in conjunction with the mass and momentum equations.

The FGM Chemical Reduction Method

The FGM chemical reduction method is used to generate the laminar flamelet database. The mixture fraction and the reaction progress variable are used to characterize mixing and chemistry respectively similar to the work of Ramaekers et al. [Ramaekers, 2005]. Flamelets are obtained using open-source suite of tools called Cantera, detailed description of chemical kinetic theory and the associated governing equations for a variety of systems that Cantera uses can be found in [Cantera Software]. Among the models that Cantera provides for steady-state, quasi-one dimensional reacting flows, freely-propagating premixed laminar flames are used for flamelet calculations.

Additional variables such as reaction progress variable and its source term are added to the database for each flamelet. After a detailed assessment, the reaction progress variable is defined as:

$$\boldsymbol{Y_c = Y_{CO_2}/\mathcal{M}_{CO_2} + Y_{H_2O}/\mathcal{M}_{H_2O}}$$

where mass fractions of species are represented with $\boldsymbol{Y}$ while weight coefficients based on the molecular weights of the corresponding species are shown by $\boldsymbol{\mathcal{M}}$. Cantera's grid refinement option is used for the flamelet calculations; however, all the flamelets are interpolated into a homogeneous space which is defined by normalized progress variable $\boldsymbol{c} \in [\boldsymbol{0}, \boldsymbol{1}]$ and $\boldsymbol{c(Z)} = (\boldsymbol{Y_C - Y_{c,min}(Z)})/(\boldsymbol{Y_{c,max}(Z) - Y_{c,min}(Z)})$.

The source term for the species included in the reaction progress variable definition is calculated as:

$$\boldsymbol{\dot{\omega}_c = \dot{\omega}_{CO_2} + \dot{\omega}_{H_2O}}$$

This term is needed as the transport equation for the reaction progress variable contains a chemical source term which is different from the transport equation for mixture fraction. In

Figure 1 contours of the reaction progress variable source term is given as it is obtained from flamelets (a single flamelet provides a line for a fix mixture value).

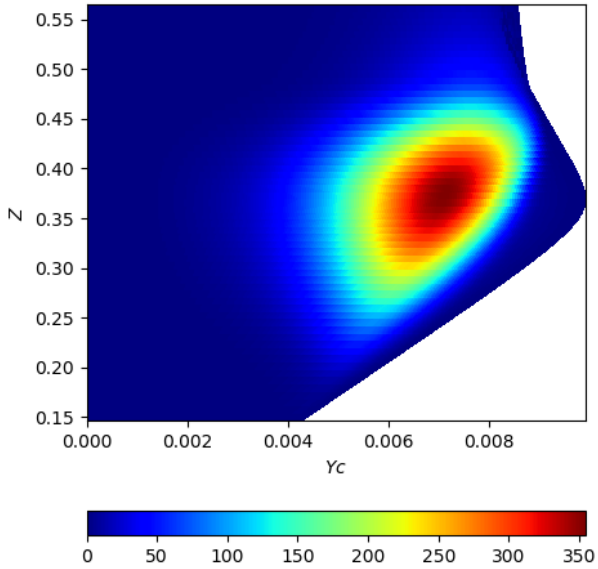

Figure 1 FGM for the source for reaction progress variable $[\boldsymbol{kg/m3/s}]$ for the flamelets within the flammability limits. The manifold consists of 113 flamelets each discretized in 101 points.

Once the flamelets within the flammability limits are calculated, species mass fractions and temperature of the flamelets outside of these limits are interpolated in order to complete mixture fraction space of the laminar flamelet database. The density of the interpolated flamelets are calculated from mass fractions and temperature values obtained with interpolation.

The Turbulence-Chemistry Interaction Method

The presumed β-PDF method is used to model the turbulence-chemistry interaction. In this method a look-up database is constructed for turbulent combustion from pre-calculated laminar flamelet database. As mentioned, it is assumed that all variables can be defined as function of mixture fraction $\boldsymbol{Z}$ and normalized reaction progress variable $\boldsymbol{c}$.

Therefore, a Favre averaged variable can be calculated as

$$\widetilde{\boldsymbol{\varphi}} = \int_0^1 \int_0^1 \boldsymbol{\varphi}(\boldsymbol{Z},\boldsymbol{c})\widetilde{\boldsymbol{P}}(\boldsymbol{Z},\boldsymbol{c})\boldsymbol{dZdc}$$

if variables are described stochastically by mass-weighted PDF's $\widetilde{\boldsymbol{P}}(\boldsymbol{Z},\boldsymbol{c})$. Additionally, $\widetilde{\boldsymbol{P}}(\boldsymbol{Z},\boldsymbol{c}) = \widetilde{\boldsymbol{P}}(\boldsymbol{Z})\widetilde{\boldsymbol{P}}(\boldsymbol{c})$ assuming $\boldsymbol{Z}$ and $\boldsymbol{c}$ statically independent.

This work follows assumptions of Ramaekers et al. [Ramaekers, 2005] to complete the PDF closure and uses $\boldsymbol{\beta}$-distribution as the assumed PDF shape. Once the weights are set for the species, all Favre-averaged variables can be defined by a combination of mean mixture fraction $\widetilde{\boldsymbol{Z}}$, mixture fraction variance $\boldsymbol{Z''}$, mean reaction progress variable $\tilde{\boldsymbol{c}}$ and reaction progress variable variance $\boldsymbol{c''}$.

RESULTS

In this section, the predictive capability of the new solver for the non-premixed, premixed and partially premixed turbulent flames is demonstrated on non-swirling and swirling conditions. Here the results are calculated in the RANS context, and the results will the LES context will be presented at the companion paper.

The non-premixed Sandia-D flame

In this section, the predictive capability of the new solver under non-premixed combustion condition is demonstrated using Sandia-D flame. The radial profiles of temperature calculated using the new solver are presented by comparing with experimental measurements *[Barlow et al. 1998]* as well as the numerical results calculated by Fluent 18.1 in Fig. 2. The results from the new solver are in good agreement with the experimental measurement at different distances to jet exit. Although the results from the new solver and Fluent have a similar trend, those from the present solver have a better agreement with experiment.

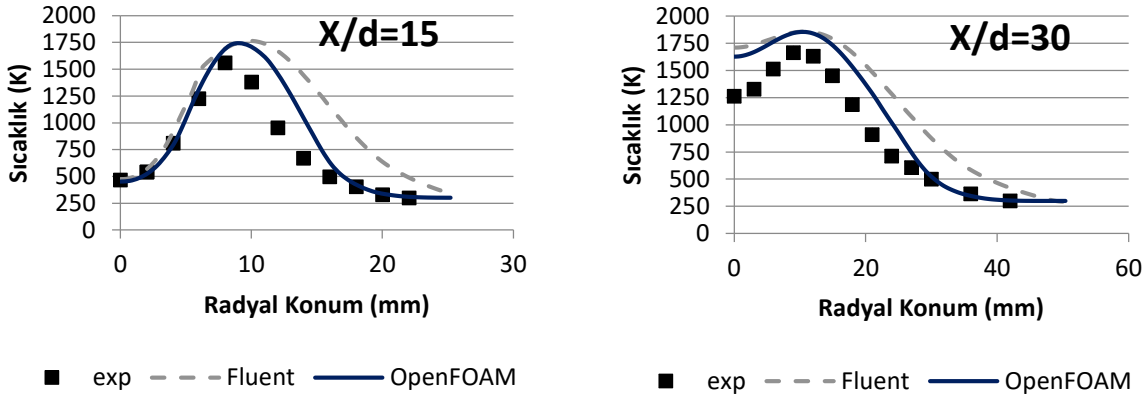

Figure 2 The temperature profiles in Sandia D flame at x/d=15 (left) and x/d=30 (right). The dots: experimental measurements, solid line: the results calculated with the present solver, the dashed line: the results calculated with Fluent.

The Cambridge-Sandia stratified flames

In this section, the numerical results for the non-swirling premixed, SwB3, non-swirling partially premixed, SwB5, and swirling premixed, SwB3, flames from Cambridge-Sandia stratified flame series are presented. The radial profiles of temperature from SwB3, SwB5 and SwB3 are presented in Figure 3-5, respectively. The numerical results are in very good agreement with the experimental measurements on non-swirling condition for both premixed and partially premixed flames. The temperature profiles under swirling condition are overall in good agreement with the measurements. However, they are over estimated close to the centreline, this may be due to the under estimate recirculation zone which prevents the cold coflow to enter the centre of the recirculation zone.

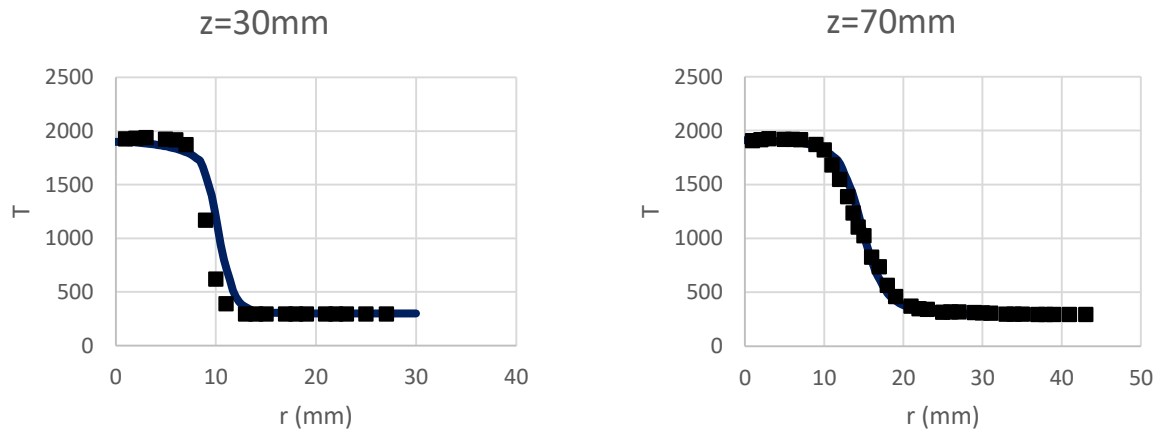

Figure 3 The temperature profiles in SwB3 flame at z = 30mm (left) and z=70 mm (right). The dots: experimental measurements, solid line: the results calculated with the present solver.

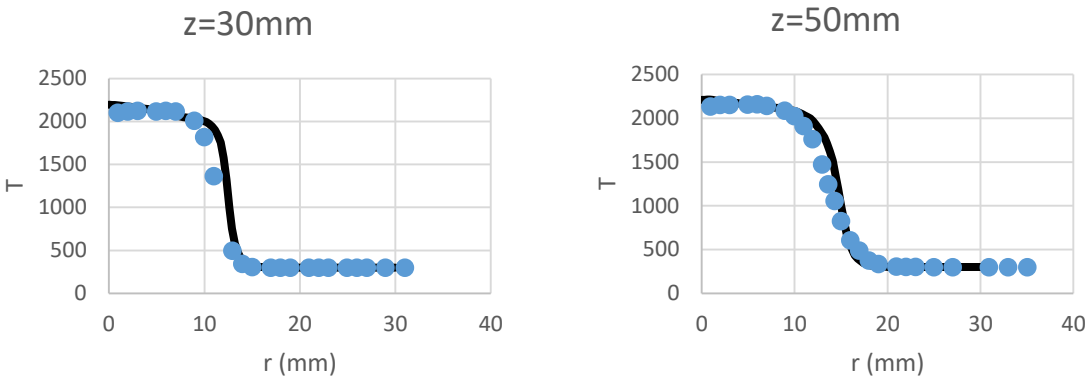

Figure 4 The temperature profiles in SwB5 flame at z = 30mm (left) and z=50 mm (right). The dots: experimental measurements, solid line: the results calculated with the present solver.

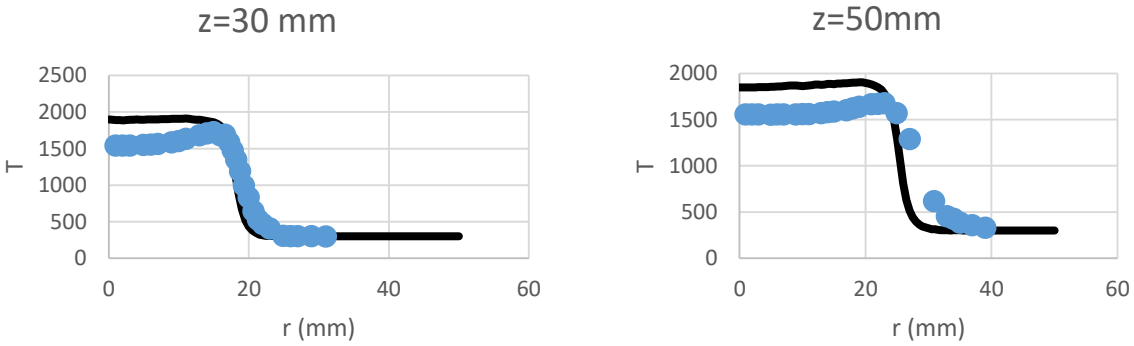

Figure 5 The temperature profiles in SwB3 flame at z = 30mm (left) and z=50 mm (right). The dots: experimental measurements, solid line: the results calculated with the present solver.

CONCLUSION

A new FGM/PDF solver is developed in OpenFOAM for the simulation of turbulent reacting flows. The predictive capability of the solver is demonstrated for both non-premixed, premixed and partially premixed turbulent flames. The results for non-premixed turbulent flames are also compared with those from Fluent. The results with the new solver for both non-premixed, premixed and partially premixed turbulent flames are in very good agreement with the experimental results, which demonstrates an efficient implementation of the FGM/PDF method within an open-source platform of OpenFOAM.

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