DEVELOPMENT AND VALIDATION OF MULTI-STAGE FGM METHOD



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Introduction

Most of the energy need in the world is met by the combustion of fossil fuels. Due to the environmental effects, more efficient combustion systems with less emissions are desired. One of the ways to analyze and design such systems is via numerical simulations. Even though direct numerical simulation (DNS) with detailed chemistry can provide all the required information about a combustion system, it is still out of reach for practical cases due to immense computational demand. For this reason, reliable computational models for turbulence, molecular diffusion, and chemistry must be developed and employed.

Among various chemistry reduction techniques, flamelet based chemistry tabulation methods such as flamelet/progress variable (FPV), flame prolongation of ILDM (FPI), and flamelet generated manifolds (FGM) have attracted attention for their successful application to various combustion systems. In these methods, it is assumed that composition space can be represented by a few controlling variables (CV). For non-premixed combustion, general practice is to select mixture fraction (Z) as the first CV to represent the molecular mixing between the fuel and oxidizer, and to select a suitable progress variable (PV) to represent the reaction progress [1-3]. However, determination of which species to use for PV definition is not always straightforward.

The traditional definition of PV includes reactant and/or product species since they are either consumed or produced during the whole process [1, 2, 4]. However, when the combustion takes place in various distinct stages, the classical choice of PV might not represent the reaction progress uniquely. An example of such a system is MILD combustion, where initially a preignition stage takes place, followed by autoignition and oxidation reactions. During the preignition stage, precursors are formed but the reactants and products do not vary much [5]. After the autoignition, fast oxidation reactions dominate and the product species are formed in large amounts, while the precursors are consumed. In some engine studies [6], precursor species were added to the definition of PV in order to represent the preignition stage, but this deteriorates the prediction capabilities in the oxidation stage since precursors are consumed.

In this study, we have developed a multi-stage (MuSt) FGM method where different stages of a combustion system are represented by different PVs,

without increasing the dimension of the FGM tables. In the following sections; details of MuSt-FGM are explained, results for a test case are presented, and finally some conclusions are drawn.

MuSt-FGM Method

As described in the Introduction section, MuSt-FGM approach is based on representing different stages of combustion using different PVs. Although the basic idea is simple, the application is not straightforward. The first issue to be tackled is how to switch between PVs during CFD calculations. In order to prevent discontinuities in PVs in spatial or temporal domain, transport equations for all PVs are solved simultaneously. To achieve this, different tables for each PV must be created, and the source terms for all PVs must be stored in all the tables.

When there are several tables for several PVs, the question is from which table to look up the required thermo-chemical variables. To determine this table switch, certain parameters need to be chosen, and thresholds for these parameters need to be defined. In this study, we have used the values of PVs themselves as the switch-determining parameter. As for the threshold value, we have created the table for each PV using the flamelets from their corresponding combustion stage, and used the lowest value of the PV in its corresponding table as the threshold.

A specific application on MILD combustion is explained here to clarify the MuSt-FGM concept further. The combustion process is divided into two parts in the MILD system; preignition and oxidation. A precursor species for the preignition stage and a product species for the oxidation stage are selected as corresponding PVs. The table for PV1 is created using the flamelets until PV1 reaches its maximum in Z-space, and flamelets thereon are used for the table for PV2. Source terms of both PVs are stored in both tables, and transport equations for both PVs are solved during the whole CFD simulation. If the value of PV2 in a CFD simulation is below its minimum in the second table, required variables are looked up from the first table; else, they are looked up from the second table.

Results

MuSt-FGM approach has been applied to the HM1 case of Dally et al.[7], and tested in 1D. Since it was shown in [8] that this case is dominated by hydrogen chemistry, PV1 was selected as HO₂ and PV2 was se-

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lected as H₂O. For the flamelet generation, DRM19 chemistry mechanism was used and constant Lewis number approach was employed. As for the flamelet type, igniting mixing layer (IML) [9] configuration was utilized.

Maximum values of PV1 and PV2 in the whole computational domain, and maximum temperature increase in Z-space are shown in Fig. 1 for the whole simulation. It is seen that MuSt-FGM results agree perfectly with the detailed chemistry results. It is worth noting that standard FGM with a single PV failed to reproduce the detailed results with either of these PVs or any combination of them.



Figure 1. Comparison of maximum of PV1 (top), PV2 (middle), and temperature increase in Z-space for detailed and MuSt-FGM cases

Conclusions

A multi-stage (MuSt) FGM method has been developed and successfully applied for a MILD combustion case. This method is useful whenever there is a clear distinction between combustion stages, such as in autoigniting systems, two-stage ignition in diesel engines, post-oxidation zone emissions, etc. Accuracy of the predictions is improved without increasing the dimension of the FGM. The only additional computational cost of MuSt-FGM method is the additional transport equation(s) to be solved during CFD calculations.

In the future, further validation of MuSt-FGM approach will be performed using DNS.

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