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INFLUENCE OF THE SUBGRID MODELS ON COMBUSTION MODELING

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Summary Turbulent flow with combustion is modelled numerically using LES (Large Eddy Simulation) method together with the flamelet approach. The governing equations applied in this work are based on the low Mach number approximation. High order compact differences/pseudospectral discretization method is applied to guarantee accurate results. The computations are performed for Sandia D flame configuration.

Introduction

Turbulent flows with combustion are among the most difficult problems occurring in nature and in industrial applications. A common appearance and importance of such flows require their correct prediction allowing for their optimization and control. The unsteady character of the turbulence implies the use of LES method which in turn allows to obtain time dependent solutions. This work concerns the analysis of the influence of subgrid models (subgrid viscosity) used within a framework of the LES method of turbulence/combustion modelling. To be able to perform such research it is necessary to exclude the effect of the numerical dissipation and its possible influence on the subgrid viscosity. The high order compact differences/pseudospectral numerical discretization method applied in computations allows for such analysis and also guarantees very accurate results. In this short summary all quantities (if not mentioned separately) appearing in the equations have standard meaning e.g. ρ - density, u_i - velocity, etc.

Combustion modeling

In the most general case modelling of the combustion processes is very expensive computationally since together with the solution of the flow field, based on the Navier-Stokes equations, it requires solution of additional transport equations for particular N species (e.g. CO, CO2, H2O, H2, etc.) produced in chemical reactions. Furthermore, the chemical kinetics which accounts for various reactions for which it is difficult to assess their importance a priori, should also be considered as a part of the solution. From the point of view of capability of available computers, approach of this type is still impossible since the numerical code would require implementation of the equations for tens species and tens (or even several hundred) chemical reactions. An approach used in this work is based on a flamelet concept [1] which states that flame can be seen as an ensemble of laminar flamelets. The equation for the conserved scalar is used, which is refereed to as the mixture fraction and denoted wherein after as z, in the form of the simple convection-diffusion equation:

$$\frac{\partial \rho z}{\partial t} + \frac{\partial \rho u_i z}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial z}{\partial x_i}\right) \tag{1}$$

The mixture fraction is a normalized quantity ($z \in [0,1]$) and represents a local fuel to oxidizer ratio ($z = 0$ - pure oxidizer; $z = 1$ - pure fuel). The assumption that one conserved scalar is sufficient to describe thermochemical state of the flow decouples the modeling of reactive phenomena from that of flow modelling. Assuming that particular species concentration, Y_k, and temperature, T, are the functions of the mixture fraction ($Y_k(\vec{x},t) = Y_k(z(\vec{x},t),t)$, $T(\vec{x},t) = T(z(\vec{x},t),t)$) the equations for these quantities may be transformed into the mixture fraction space resulting in the equations of the form:

$$\rho \frac{\partial Y_k}{\partial t} = \dot{\omega}_k + \rho \mathcal{D}\left(\frac{\partial z}{\partial x_i}\frac{\partial z}{\partial x_i}\right)\frac{\partial^2 Y_k}{\partial z^2} = \dot{\omega}_k + \frac{1}{2}\rho\chi\frac{\partial^2 Y_k}{\partial z^2} \tag{2}$$

where $\mathcal{D}$ is the diffusion coefficient assumed the same for each species and $\dot{\omega}$ is the reaction rate depending on the chemical kinetics. The above equation together with the equation for the temperature constitute the unsteady flamelet approach in which the dependence of the temperature and species on time is retained. However, knowing that characteristic time of the chemical processes is much smaller than time of the turbulent phenomena one can assume the structure of the flamelet to be steady even though the mixture fraction itself depends on time. With this assumption, at every instantaneous time of the solution, the values of $Y_k(\vec{x})$ and $T(\vec{x})$ may be computed based on the mixture fraction. The functional dependences $Y_k(\vec{x}) = Y_k(z(\vec{x}))$ and $T(\vec{x}) = T(z(\vec{x}))$ are provided from the solution of the laminar flamelet calculations of the steady flamelet equations. Knowing the species concentration corresponding to a given value of the mixture fraction the density may be computed based on the equation of state and then also expressed as the functional dependence of z. In the context of LES method of turbulence modeling, where every quantities are represented as the superposition of their filtered and subgrid parts, the mixture fraction equation has the form:

$$\frac{\partial \bar{\rho}\tilde{z}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\rho\mathcal{D} + \frac{\mu_t}{Pr_t}\right)\frac{\partial \tilde{z}}{\partial x_i}\right) \tag{3}$$

where $\bar{(\cdot)}$ and $\tilde{(\cdot)}$ represents the LES-filtered and Favre-filtered variables, Pr_t stands for the turbulent Prandtl number and μ_t is the turbulent viscosity obtained from the subgrid model.

Flow field modeling

For the strongly variable density/temperature low speed (low Mach) flows it is necessary to take into account their spatially and temporally unsteady character. In this research we applied the so-called low Mach number approximation of the governing equations, where the flow variables are expressed as power series of $\epsilon = \gamma M^2$ (γ - ratio of the specific heats, M - Mach number) in the form: $f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \mathcal{O}(\epsilon^3)$. The LES-filtered continuity and the Navier-Stokes equations at the zero order quantities (except for the pressure) are given as:

$$\frac{\partial \overline{\rho^{(0)}}}{\partial t} + \frac{\partial \overline{\rho^{(0)}} \widetilde{u^{(0)}}_j}{\partial x_j} = 0 \tag{4}$$

$$\frac{\partial \overline{\rho^{(0)}} \widetilde{u^{(0)}}_i}{\partial t} + \frac{\partial \overline{\rho^{(0)}} \widetilde{u^{(0)}}_i \widetilde{u^{(0)}}_j}{\partial x_j} = -\frac{\partial \overline{p^{(1)}}}{\partial x_i} + \frac{\partial}{\partial x_j}\left((\mu + \mu_t)\left(\frac{\partial \widetilde{u^{(0)}}_i}{\partial x_j} + \frac{\partial \widetilde{u^{(0)}}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \widetilde{u^{(0)}}_k}{\partial x_k}\right)\right) \tag{5}$$

We note that in the framework of low Mach number approximation the equation for the mixture fraction should also be seen as an equation for zero order quantities ($\overline{\rho^{(0)}}$, $\widetilde{z^{(0)}}$). In the present work the turbulent viscosity is modelled using Smagorinsky subgrid model together with its dynamic counterpart and filtered structure function model [2].

Solution procedure and sample results

The solution procedure for the set of equations (4), (5) and (3) is based on the projection method which allows to determine the pressure field $p^{(1)}$ from the Poisson equations. The time advancement is performed by low storage III^{th} order Runge-Kutta method, all space derivatives are discretized using VI^{th} order compact differences method or Fourier pseudospectral method in the directions for which periodic boundary conditions are assumed. The preliminary results showing the contours of the mixture fraction for Sandia D flame are presented in Fig.1, they are in reasonably good agreement with experimental data. The periodic boundary conditions are applied on the boundaries parallel to the jet axis, at the outflow we applied convective type boundary conditions while at the inlet the velocity and mixture fraction profiles correspond to experimental data. These computations were performed with the filtered structure function model for the subgrid scale.

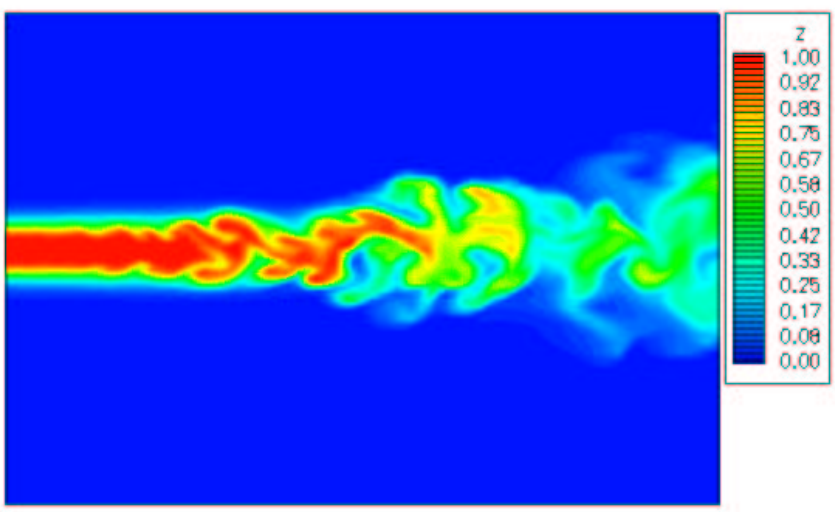

Figure 1. Mixture fraction contours in Sandia D flame.

CONCLUSIONS

This summary presents the main idea and the solution strategy for modeling turbulent flow with combustion. The obtained results are very promising, the research concerning comparison of the accuracy of various subgrid models is currently in progress.

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