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Computer simulations of combustion processes - Project

CFD simulation of gas turbine combustor - turbulence models comparison

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1 Introduction

New computational methods are continuously developed in order to solve problems in different engineering fields. One of these fields is gas turbines, where the challenge is to make gas turbines more efficient and to reduce emissions that are bad for the environment. One of the main parts of a gas turbine that can be improved is the combustion chamber. In order to optimize the combustion chamber, both experimental and numerical methods are called for. Numerical optimization implies the necessity to model the most important phenomena in combustion chambers such as turbulent swirling flow, chemical reactions, heat transfer, and so on. In this project we try to simulate these processes in a simple combustor with various turbulence models.

2 Literature: scientific background

2.1 Gas turbine combustion chamber

A combustion chamber is a component or area of a gas turbine where combustion takes place. It is also known as a burner, combustor or flame holder. In a gas turbine engine, the combustor is fed high pressure air by the compression system. The combustor then heats this air at constant pressure. After heating, air passes from the combustor through the nozzle guide vanes to the turbine.

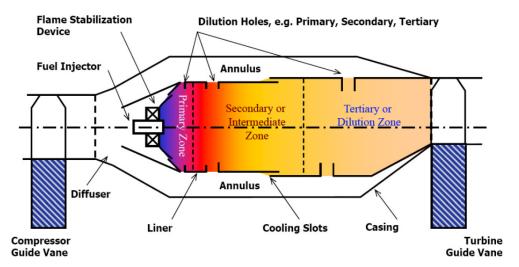


Figure 1: Combustor chamber scheme

A combustor must contain and maintain stable combustion despite very high air flow rates. To do so combustors are carefully designed to first mix and ignite the air and fuel, and then mix in more air to complete the combustion process.

Combustors play a crucial role in determining many of an engine's operating characteristics, such as fuel efficiency, levels of emissions and transient response (the response to changing conditions such as fuel flow and air speed).

2.2 Physics of Premixed Combustion

In premixed combustion, fuel and oxidizer are mixed at the molecular level prior to ignition. Combustion occurs as a flame front propagates into the unburnt reactants. Examples of premixed combustion include aspirated internal combustion engines, lean-premixed gas turbine combustors, and gas-leak explosions.

The effect of turbulence is that it wrinkles and stretches the propagating laminar flame sheet, increasing the sheet area and, in turn, the effective flame speed. The large turbulent eddies tend to wrinkle and corrugate the flame sheet, while the small turbulent eddies, if they are smaller than the laminar flame thickness, may penetrate the flame sheet and modify the laminar flame structure. As the premixed flame is a reaction wave propagating from burned to fresh gases, the basic parameter is known to be the progress variable. In the fresh gas, the progress variable is conventionally put to zero. In the burned gas, it equals unity. Across the flame, the intermediate values describe the progress of the reaction. A progress variable can be set with the help of any quantity, like temperature, reactant mass fraction, provided it is bounded by a single value in the burned gas and another one in the fresh gas. The progress variable is usually named c, in usual notations.

$$c = \frac{T - T_f}{T_b - T_f}$$

Where b stands for burned gas, and f stands for fresh gas. In OpenFOAM, the flame front propagation is modelled by solving a transport equation for the density-weighted mean reaction regress variable denoted by b, where:

$$b = 1 - c$$

$$\frac{\partial}{\partial t}(\rho b) + \nabla(\rho \overrightarrow{u}b) - \nabla(\frac{\mu_t}{S_{c_t}}\nabla b) = -\rho S_c \tag{1}$$

 $S_{c_t} = \frac{\mu}{\rho D}$ - turbulent Schmidt number S_c - reaction regress source term, modeled as equation:

$$\rho S_c = \rho_u S_u \Xi |\nabla b| \tag{2}$$

By substituting equation 2 to equation 1 we would have:

$$\frac{\partial}{\partial t}(\rho b) + \nabla(\rho \overrightarrow{u}b) - \nabla(\frac{\mu_t}{S_{c_t}}\nabla b) = -\rho_u S_u \Xi |\nabla b| \tag{3}$$

where:

b - mean reaction regress variable

 S_u - laminar flame speed [m/s]

D - diffusion coefficient $[m^2/s]$

 Ξ - Turbulent flame velocity and laminar flame velocity ratio

 ρ_u : density of unburnt mixture $[kg/m^3]$

Based on this definition:

b=1 - unburnt mixture

b=0 - burnt mixture

The value of b is defined as a boundary condition at all flow inlets. It is usually specified as either 0 (unburnt) or 1 (burnt). OpenFOAM has a premixed turbulent combustion model based on the reaction regress variable(b=1-c) approach. Information about this model is provided in the bEqn.H file of the XiFoam solver.

2.3 Turbulence modeling

The main goal of this project is to compare various turbulence models. From among many available models I choose the most popular one from the main groups, which are $k-\epsilon$, $k-\omega$ and Large Eddy Simulation(LES). Models of my choice are "standard" $k-\epsilon$ model, SST $k-\omega$ model and Smagorinsky Large Eddy Simulation model. Below there is a brief description of each of them.

2.3.1 Standard k- ϵ model

The k- ϵ model is one of the most common turbulence models. It is a two equation model, that means, it includes two extra transport equations to represent the turbulent properties of the flow. This allows a two equation model to account for history effects like convection and diffusion of turbulent energy.

The first transported variable is turbulent kinetic energy, k. The second transported variable in this case is the turbulent dissipation, ϵ . It is the variable that determines the scale of the turbulence, whereas the first variable, k, determines the energy in the turbulence.

There are two major formulations of $k-\epsilon$ models. That of Launder and Sharma is typically called the "Standard" $k-\epsilon$ Model. The original impetus for the $k-\epsilon$ model was to improve the mixing-length model, as well as to find an alternative to algebraically prescribing turbulent length scales in moderate to high complexity flows.

The k- ϵ model has been shown to be useful for free-shear layer flows with relatively small pressure gradients. Similarly, for wall-bounded and internal flows, the model gives good results only in cases where mean pressure gradients are small; accuracy has been shown experimentally to be reduced for flows containing large adverse pressure gradients.

Turbulent viscosity is modelled as:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$$

2.3.2 SST k- ω model

The SST k- ω turbulence model is a two-equation eddy-viscosity model which has become very popular. The shear stress transport (SST) formulation combines the best of two worlds. The use of a k- formulation in the inner parts of the boundary layer makes the model directly usable all the way down to the wall through the viscous sub-layer, hence the SST k- ω model can be used as a Low-Re turbulence model without any extra damping functions. The SST formulation also switches to a k- ϵ behaviour in the free-stream and thereby avoids the common k- ω problem that the model is too sensitive to the inlet free-stream turbulence properties.

The SST $k-\omega$ model behaves well in adverse pressure gradients and separating flow. The SST $k-\omega$ model does produce a bit too large turbulence levels in regions with large normal strain, like stagnation regions and regions with strong acceleration. This tendency is much less pronounced than with a normal $k-\epsilon$ model though.

2.3.3 Smagorinsky Large Eddy Simulation model

Large eddy simulation (LES) is a popular technique for simulating turbulent flows. An implication of Kolmogorov's (1941) theory of self similarity is that the large eddies of the flow are dependent on the geometry while the smaller scales more universal. This feature allows one to explicitly solve for the large eddies in a calculation and implicitly account for the small eddies by using a subgrid-scale model (SGS model).

Mathematically, one may think of separating the velocity field into a resolved and sub-grid part. The resolved part of the field represent the "large" eddies, while the subgrid part of the velocity represent the "small scales" whose effect on the resolved field is included through the subgrid-scale model. Formally, one may think of filtering as the convolution of a function with a filtering kernel G:

$$\overline{u_i}(\overrightarrow{x}) = \int G(\overrightarrow{x} - \overrightarrow{\xi}u(\overrightarrow{\xi})d\overrightarrow{\xi}) d\overrightarrow{\xi}$$
 (4)

resulting in

$$u_i = \overline{u_i} + u_i'$$

where $\overline{u_i}$ is the resolvable scale part and u_i' is the subgrid-scale part.

In the Smagorinsky model, the eddy viscosity is modeled by :

$$\mu_{sgs} = \rho (C_s \Delta)^2 |\overline{S}|$$

3 Model

3.1 OpenFOAM

I'm running a simulation using the XiFoam solver included in the OpenFOAM package. XiFoam, is a solver for compressible premixed/partially-premixed combustion with turbulence modelling, therefore it completely meets my requirements.

OpenFOAM or "Open Field Operation and Manipulation" is a CFD toolbox written in C++, used primarily to create executables, known as applications. The

applications fall into two categories 1) solvers and 2)utilities. Solvers are each designed to solve a specific problem in continuum mechanics; and utilities, are designed to perform tasks that involve data manipulation. The OpenFOAM distribution contains numerous solvers and utilities capable of solving anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetism. It also includes tools for meshing, notably snappyHexMesh - a parallelised mesh generation tool for complex CAD geometries, utilities for post-processing and data manipulation. The overall structure of OpenFOAM is shown in fig.2 . Almost everything (including mesh generation and post-processing) runs in parallel as standard, enabling users to take full advantage of the computer hardware at their disposal.

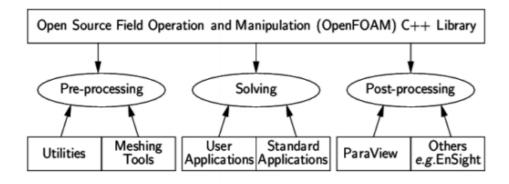
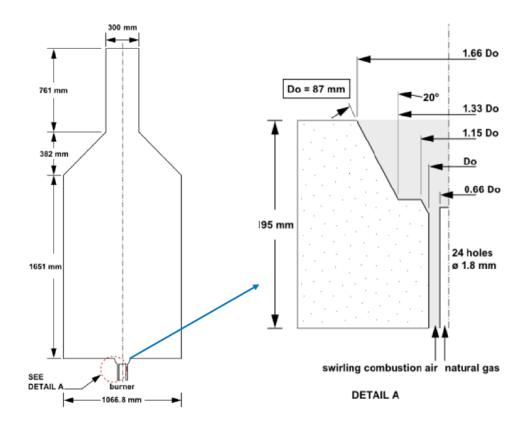


Figure 2: OpenFOAM applications: solvers and utilities

3.2 Geometry and mesh

Due to keeping calculations on my own computer and hence the low computing power, I decided to use a very simplified geometry of the combustion chamber. I took the geometry directly from the ANSYS Fluent Combustion Modeling Workshop (it is shown in the fig.3). It is a 2D, axis-symmetric mesh containing 10233 cells. I decided to ignore a natural gas inlet to be able to run a premixed gas simulation. Rest of the combustor is exactly like we can see in fig.3



 ${\bf Figure~3:~Combustion~chamber~geometry}$



Figure 4: Geometry transformed into mesh

4 Results

As the results of the simulation, I put screen shots from the ParaView post-processing program, showing the fields of temperature, velocity and pressure in various time steps. The figures show different turbulence models juxtaposed with each other, respectively from above: Launder and Sharma ("standard") k- ϵ , SST k- ω and Smagorinsky LES.



Figure 5: $k-\epsilon$ temperature field at time=0.01s



Figure 6: k- ω temperature field at time=0.01s



Figure 7: LES temperature field at time=0.01s

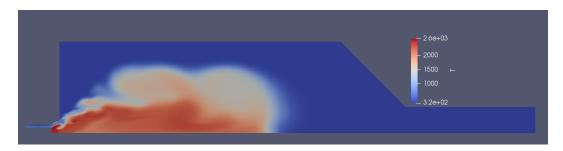


Figure 8: k- ϵ temperature field at time=0.05s

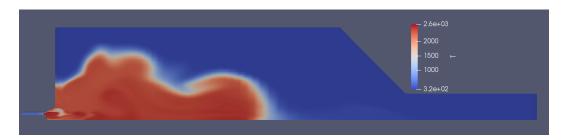


Figure 9: k- ω temperature field at time=0.05s

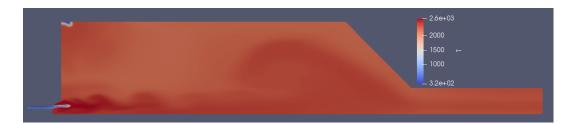


Figure 10: LES temperature field at time=0.05s



Figure 11: k- ϵ temperature field at time=0.1s

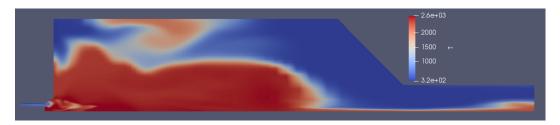


Figure 12: k- ω temperature field at time=0.1s

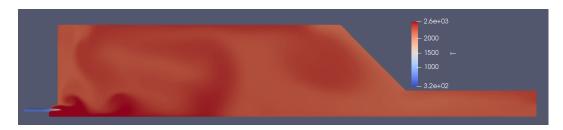


Figure 13: LES temperature field at time=0.1s



Figure 14: k- ϵ pressure field at time=0.01s



Figure 15: k- ω pressure field at time=0.01s



Figure 16: LES pressure field at time=0.01s



Figure 17: k- ϵ pressure field at time=0.05s



Figure 18: k- ω pressure field at time=0.05s

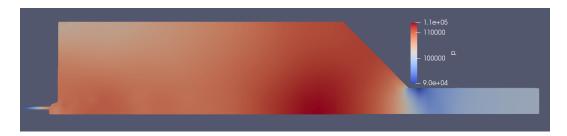


Figure 19: LES pressure field at time=0.05s

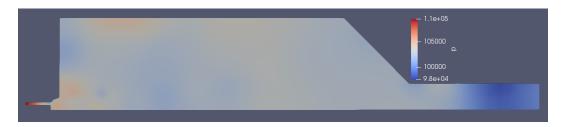


Figure 20: k- ϵ pressure field at time=0.1s



Figure 21: k- ω pressure field at time=0.1s



Figure 22: LES pressure field at time=0.1s



Figure 23: k- ϵ velocity field at time=0.01s



Figure 24: k- ω velocity field at time=0.01s



Figure 25: LES velocity field at time=0.01s



Figure 26: k- ϵ velocity field at time=0.05s



Figure 27: k- ω velocity field at time=0.05s



Figure 28: LES velocity field at time=0.05s

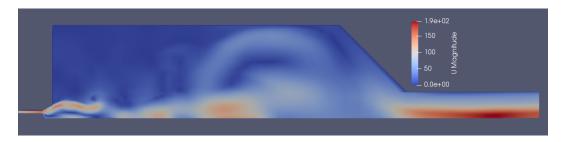


Figure 29: k- ϵ velocity field at time=0.1s

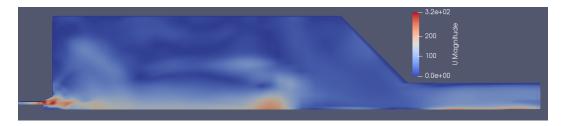


Figure 30: k- ω velocity field at time=0.1s



Figure 31: LES velocity field at time=0.1s

5 Conclusion

Despite the fact that you can clearly see the differences between individual turbulence models, it is difficult to say which one works best without a specific reference level.

To really check the reliability of these models, we should run simulations using the geometry of "real" combustion chamber and validate the results with experimental measurement data. It is because the purpose of these simulations is to closely imitate the actual physical phenomena occurring in combustors which can not be achieved without comparison with experimental data.

6 Sources

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