Improved numerical modelling for Chemically Reactive, Turbulent Supersonic Flows

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Overview

For many decades now newspapers have periodically talked about how close we are to building "hypersonic" planes that would fly at several times the speed of sound. Such vehicles would be able to connect, say, Europe and Australia in four hours and they would represent the greatest advance in the aviation industry since the introduction of jet engines over sixty years ago. Unfortunately, we are not as close to developing sustained hypersonic flight as is sometimes portrayed in the news. Much work is still needed in many areas such as drag reduction, thermal protection and materials science. But the most challenging issues lie in the development of the engines that would propel these hypersonic planes. When a vehicle is flying in the atmosphere at such high velocities, the combustion between the fuel and the stream of air inside the airplane's engines has to occur at supersonic speeds. Under these conditions, achieving a complete and stable combustion is much more challenging due to the presence of shock waves that interact with the turbulent flow field and with the flame. In addition, higher speeds mean that the gas will spend less time inside the combustor and that makes it much more difficult to achieve a good mixture - and thus an efficient combustion - between the fuel and the air.

Both the inherent difficulties as well as the important applications it would have in the civil and military aerospace industries make high-speed turbulent combustion currently an area of very active research. Unfortunately, due to the particularly harsh conditions present in the combustor, experimental testing in wind tunnels can only provide limited quantitative measurements and is very expensive. Computer simulations, on the other hand, provide a huge amount of data about the flow-field and are relatively cheap to run. The basic idea behind these simulations is to subdivide the physical space into a discrete (and finite) number of points and solve the equations of fluid dynamics on these points only. An example of the results that can be obtained is shown on Fig. 1.

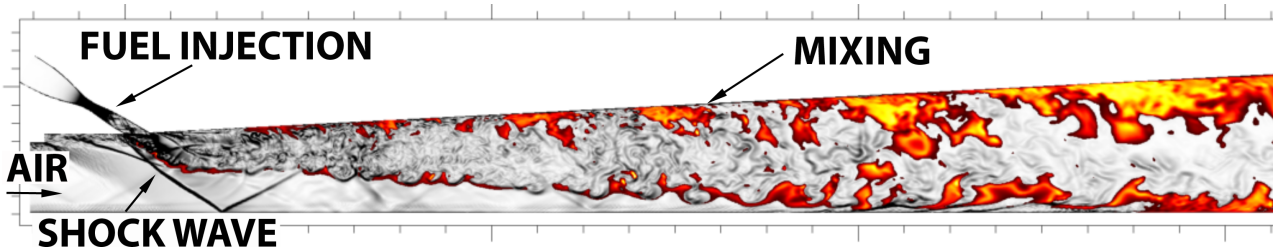

Figure 1: Numerical simulation of a supersonic combustor. On the top left it can be seen the oblique fuel injector. Red and yellow areas indicate where combustion is taking place.

The main issue with the computational approach is that turbulent flows contain many fluid structures that are characterized by different sizes (or scales) and it is very hard to simulate all of them. This is certainly true for high-speed turbulent flows, for which the range of scales (between the largest and the smallest structures) is so large that the number of points required

to completely resolve all the features of the flow greatly exceeds the computational resources that are available at the moment. Even extrapolating from the current growth of computing speed (and assuming it won't slow down), these types of "high-resolution" simulations will be impossible for at least the next fifty years [1]. The best alternative available is to use a smaller number of discrete points that resolve only the largest scales of the flow, usually called eddies. The effect of the smaller scales (which are called sub-grid scale (SGS) terms) are evaluated using a model. This approach is called Large Eddy Simulation (LES) and it has proven to be very successful for non-reacting flows, where well established, universal, models for the SGS terms are available. This is not the case when chemical reactions are considered, as the additional chemistry terms in the fluid-dynamics equations are strongly dependent on the particular type of reaction and thus far from being universal. As a consequence, in many practical simulations, the chemical SGS terms are either neglected or evaluated using empirical, problem-dependent models. This approach greatly reduces the predictive capabilities of the simulation and there are numerous cases where it has been shown to provide inaccurate solutions [2].

My research addresses this issue by considering a novel stochastic methodology that is able to fully evaluate the chemical SGS source terms without the need for any type of model. Physically, the chemical source terms depend on the local temperature and the local chemical concentration and are highly non-linear. The main idea underlying this new methodology is to consider the entire statistical distribution of both the temperature and the concentration and use this information to compute the chemical source terms. Unlike conventional LES, where only the mean temperature and concentration are used, this strategy allows to directly take into account the effects of all the flow scales on the chemistry terms, thus eliminating the need to model the small scale interactions. The statistical distribution of a physical variable is called, in this context, the Filtered Mass Density Function (FMDF) [2]. The FMDF of the chemical concentration and the temperature can be obtained by solving a transport equation which governs the evolution of the FMDF in space and time. As the FMDF is not a single variable but actually a mathematical distribution, solving its transport equation using traditional deterministic numerical methods would be impractical. Instead, probabilistic Monte Carlo techniques, which work out the solution by using a large number of particles in the flow field, are employed. Since FMDF methods only solve for the temperature and chemical concentration, they have to be used in conjunction with a conventional fluid dynamic solver that is able to provide the other physical quantities in the flow (namely the velocity field and the pressure).

Although the focus of my research will be mainly on supersonic combustion for hypersonic vehicles propulsion, this new methodology can be applied to any type of turbulent, chemically reactive flow. Examples include important areas such as internal combustion engines, power generation and modelling of chemical reactors. In addition, it has been recognized that chemical reactions play an major role in boundary layer stability which, in turns, greatly affects the aerodynamic drag of supersonic vehicles. A better understanding and quantification of these mechanisms would be a further step forward towards the achievement of sustained hypersonic flight.

References

[1] Choi H., Moin P., "Grid-point requirements for Large Eddy Simulation: Chapman's estimates revisited", *Phys. Fluids*, 24, 011702 (2012).

[2] Jaberi F. A. et al., "Filtered Mass Density Function for Large-Eddy Simulations of Turbulent Reacting Flows," *J. Fluid Mech.*, Vol. 401, (1999) pp. 85–121.