

Direct simulation of compressible reacting flows

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Summary

A research program for direct numerical simulations of compressible reacting flows is described. Two main research subjects are proposed: the effect of pressure waves on turbulent combustion and the use of direct simulation methods to validate flamelet models for turbulent combustion. The interest of a compressible code to study turbulent combustion is emphasized through examples of reacting shear layer and combustion instabilities studies. The choice of experimental data to compare with direct simulation results is discussed. A tentative program is given and the computation cases to use are described as well as the code validation runs.

1. Introduction

A considerable part of progress to be made in future years in the field of turbulent combustion studies might be achieved through direct simulation methods. These methods have already demonstrated their possibilities in the case of non-reacting flows, and there is little doubt that they will be as powerful in the case of reacting flows. However, such progress will require considerable improvements of existing direct simulation codes to account for specific phenomena occurring in reacting flows. One of the most important issues in this field is to take into account the compressibility effects. This should be done at different levels by incorporating the following effects:

- 1- *density variations generated by heat release*
- 2- *acoustic waves*
- 3- *strong compressibility effects due to high relative Mach numbers*

These three steps represent growing complexity. It is rather obvious that *density variations* generated by heat release strongly modify the velocity field and the strain rates, changing the turbulent field and, therefore, the combustion rate itself. Therefore, direct simulations aimed at studying cold flames (essentially flames with constant density) can not predict the behavior of real flames. This does not mean that these simulations are not interesting: they retain many features of real flames like chemical and diffusive mechanisms. Building a code for direct simulation of flames with non constant density does not necessarily mean using a compressible code. Random vortex methods as well as spectral methods can provide such capacity without taking compressibility effects into account (Ghoniem and Sethian 1987, Riley et al 1986, Givi and Metcalfe 1986).

Nevertheless, ability to include compressibility is highly desirable because it fulfills not only criterion 1 but also the two others: computing acoustic waves and mean pressure gradients.

Experimental results suggest that *acoustic waves* are of primary importance for combustion problems (Poinsot et al 1986, Darabiha et al 1985) but also for non-reacting flows. Non-reacting shear layers exhibit phenomena where acoustic waves play an important role by introducing a feedback loop through which phenomena occurring downstream (for example a vortex coalescence) can send information upstream (to the vortex shedding region) and create a locking phenomenon (Ho and Huerre 1984, Ho and Huang 1982). This locking may be weak or strong. We will call it weak when it does not lead to an instability where the acoustic field becomes intense. This is the case in most ducted shear layers. It should not be concluded that *weak coupling means no effect of acoustic waves*: even if the acoustic field is not intense, vortex shedding can be very sensitive to pressure waves, and this point is seldom taken into account in direct simulation methods.

In non-reacting shear layers the coupling may become strong as, for example, in the case of the edgetone experiment. Placing an obstacle in the shear layer can amplify the acoustic feedback and lead to the production of a highly coherent and intense sound generated by the coupling between coherent structures in the shear layer, their impact on the obstacle, and the acoustic waves in the flow (Ho and Nosseir 1981, Tang and Rockwell 1983, Knisely and Rockwell 1982).

When combustion takes place, the coupling is even enhanced by the reaction taking place in the flow structures. Experimentally, this coupling is strong enough in many situations to induce very large oscillations of all the flow parameters and lead to complete extinction by blow off or flash back of the flames. Although it does not always lead to such extreme instabilities, we have to suppose that this coupling can be an important part of the global behavior of turbulent reacting flows and, therefore, incorporate acoustic waves in our model.

It is possible to ask whether we really need direct simulation codes to study interactions between combustion and acoustic waves and whether we could simplify the problem and for example assume that acoustic waves and turbulence act independently on the flow. Acoustic waves in usual systems have large wavelengths compared to the reaction zone thickness, and we might try to disconnect the effects of pressure waves and those of turbulence. Such attempts have been made to compute combustion instabilities in the 'Thin Flame' models proposed by Yang and Culick (1986) or Poinsot and Candel (1988). In these models the interaction between combustion and turbulence is represented simply by a turbulent flame speed while all interactions between the flame movements and the acoustic field are explicitly computed. Poinsot and Candel (1988) show that these models are unable to predict any turbulent combustion instability if the turbulent flame speed does not depend on the local turbulence or on the local

pressure. This shows that pressure waves and turbulence have strong interactions and that this coupling must be explicitly taken into account. This requires the use of a direct simulation code (for turbulence estimation) which must be compressible (for acoustic waves computation).

The last case requiring compressible computations is clearly obtained for flows exhibiting *high relative Mach numbers* such as supersonic reacting flows. Compressibility is not limited to the flow perturbations (as it was for acoustic waves) in these cases but is a basic characteristic of the mean flow itself. Compressible calculations are obviously required for this situation.

Looking at all these cases is far beyond the scope of this work. Therefore, I have chosen to concentrate this study on two generic cases of compressible reacting flows which offer a very wide range of interests:

- ▷ *Effect of acoustic waves on reacting and non-reacting shear flows*
- ▷ *Validation of flamelet models for turbulent combustion*

2. Effect of pressure waves on turbulent combustion

Acoustic waves play an important role in non-reacting as well as reacting flows. As most experiments are performed in ducts, the acoustic modes of these ducts are first choice candidates to excite the flow to study. Therefore, many experimental shear layers are controlled mainly by acoustic excitations (Ho and Huerre 1984). We will start this work by looking at the effects of acoustics in the non-reacting mixing layer and afterwards proceed to the reacting case. In these two situations, the questions addressed will be essentially the same:

- How should excitation be introduced in the direct simulation to correspond to experiments? Exciting the shear layer at its most amplified hydrodynamic frequency is clearly not compatible with all experimental data: many experiments exhibit a sensitivity to acoustics that must be considered (Masutani et al 1986, Poinso et al 1987). Exciting the flow with an acoustic frequency of the duct might be an interesting alternative, but the best technique would be to introduce initial perturbations on different oscillation modes (acoustic and random modes) and let the system evolve without other excitation (Poinso and Candel 1988). The use of reflecting boundary conditions for acoustic waves should insure that the flow keeps being excited by its own oscillations. It is interesting to note that this method has already been used successfully to predict coalescence in free shear layers (Grinstein et al 1987) and theoretically confirm the feedback law proposed by Laufer (see Ho and Huerre 1984).

- What acoustic modes are involved in the locking phenomena?

- How does the flow respond to acoustic excitations, and what kind of locking can be isolated from the results? For this study, the reacting case might be simpler than the non-reacting case because of generation of acoustic disturbances by non steady combustion in vortices.

Many experiments have been conducted on shear layers and could be used to validate the results obtained from direct simulation. After a preliminary study,

however, the experiment of Masutani and Bowman (1986) on a reacting shear layer appears as a good choice because it was performed in the premixing domain where three dimensional effects are reduced and for Reynolds numbers which are accessible to direct simulation. All computations will be two dimensional. One of the streams will contain nitrogen and nitric oxide while the other contains nitrogen and ozone. Either reactant (nitric oxide or ozone) can be injected in the high speed side. The Reynolds number based on the vorticity thickness and the velocity difference will vary between 300 and 2000. The chemistry can be represented by only one reaction namely:



This paper provides many experimental data such as mean profiles, RMS profiles, PDFs and power spectra density at different locations for reacting and non reacting cases. These data should constitute a good and critical basis for code testing.

3. Validation of flamelet models for turbulent combustion

Flamelet models for turbulent combustion are the subject of growing interest. In these models, turbulent combustion is modelled as a collection of small laminar flamelets which are convected, stretched, and quenched by turbulence without losing their laminar structure. These assumptions allow a computation of the mean turbulent reaction rate using only two informations:

- 1- the laminar flame speed of the flamelets
- 2- the topology of the flamelets ensemble

Computing the laminar speed and the extinction limits of stretched flames has become a relatively easy task (Giovangigli and Smooke 1987) and different data bases giving flame speeds for various flow parameters are or will be available in the near future. Defining the topology of the flamelets is a much more difficult task and constitutes the basic problem of flamelet modelling.

A powerful flamelet model has been proposed by Marble and Broadwell (1977) and developed by S. Candel and coworkers (1988) (see also Darabiha et al 1987). In this model called the *Coherent Flame Model (CFM)* the topology of the flamelets is described only by their surface Σ , the flame front surface per unit mass of gas (the flame front surface per unit volume of gas $\rho\Sigma$ is more convenient to use). This approach requires the chemical time to be smaller than the turbulent times so that the flame is essentially wrinkled and stretched by turbulence but that it remains a continuous interface separating burnt and fresh gases. An equation is written for this flame surface and coupled with the flow properties: turbulence field, chemical data, etc. The laminar flame speed is obtained from a data base containing computations of strained laminar flames at stagnation point with complete chemistry. The interesting feature in the model is its ability to handle chemical problems on one side to obtain the local flame

speed of the flamelets and the turbulence-combustion interaction on the other side through the flame surface equation. Although the CF model has already been successfully applied in different practical combustion systems, its complete validation will certainly be easier if direct simulation is used to ascertain most of the assumptions made to obtain the *flame surface equation*. This equation describes the evolution of the flame surface in each computational cell. Like the equations derived in turbulence modelling for the turbulent kinetic energy or the dissipation rate, this equation requires modelling of many physical mechanisms (Marble and Broadwell 1977, Candel et al 1988):

- convection of the flamelets by the mean flow
- diffusion of the flamelets by turbulence
- flamelet stretching by the turbulent field (which is a source term for the flame surface equation)
- annihilation of flamelets by mutual interactions (which is a sink term for the flame surface equation).

$$\frac{\partial \rho \Sigma}{\partial t} + U \frac{\partial \rho \Sigma}{\partial x} + V \frac{\partial \rho \Sigma}{\partial y} = \mathbf{E} \rho \Sigma + \text{Diffusion Term} - \text{Annihilation Term}$$

The term $\mathbf{E} \rho \Sigma$ represents the flame surface increase due to the stretching of the flame front by the turbulent flow and is the dominant term in the flame surface equation. \mathbf{E} is the stretch rate and might be easily obtained as $\sqrt{\varepsilon/\nu}$ if chemistry was infinitely fast and the flame was an infinitely thin interface (ε is the turbulent dissipation rate and ν is the kinematic viscosity). This is not the case, and because of chemical effects, most flamelets will be quenched if they are submitted to high stretch rates. Therefore, one of the first difficulties is to give a proper estimate of \mathbf{E} taking into account all possible interactions between the flame front and the turbulent field. Assumptions are usually made for each of these terms, but very few validations of these hypotheses exist. For example, Marble and Broadwell (1977) estimated \mathbf{E} in a reacting shear layer to be of the order of $\frac{\partial U}{\partial y}$ which is a proper estimate of the stretch rate of the large eddies in the layer but does not include any chemical effects. The interaction of a laminar flame and a vortex has already been studied analytically (Cetegen and Sirignano 1987) and numerically (Candel and Laverdant 1987) but recent direct simulation results performed on the structure of premixed flames interacting with a vortex show more complete and promising results (Rutland and Ferziger 1989).

We intend to extend these studies to test and improve some of the modelling assumptions used in flamelet models by studying simple interactions between a laminar flame front and an imposed vorticity field. This will be done on a diffusion flame in a shear layer or on a laminar premixed flame propagating in a duct and submitted to a vortex. In these two cases, the initial flame structure will be that of a laminar flame and the objective will be to study how this structure interacts with the vorticity field generated by the shear layer or by

the isolated vortex. The flame surface will be tracked and compared to the computation given by the flame surface equation of the CF model using the same input values for strain rates. The computations will be two dimensional. The main parameters will be the Damkohler number based on the chemical time and the roll up time of the eddy. Following problems will be more precisely considered:

- In which range of Damkohler numbers does the initial flame retain its laminar structure? (In other words can we use the flamelet concept to describe turbulent combustion at this Damkohler number?)

- What are the local values of the strain rates, and is there any evidence of flame extinction by strain?

- How must the CF model equation for the flame surface be modified to predict correctly results given by the direct simulation? How is the effective stretch rate E given by the direct simulation related to the flow vorticity and to the flame chemical time?

- What is the effect of eddies smaller than the flame front thickness? (High values of Damkohler numbers). Can the flamelet concept be extended to regimes where turbulence does not only wrinkle and stretch the flame but also thickens it?

One may note that acoustic waves are not a first order phenomenon in this part of the work but that variable density effects certainly are. Density variations will affect the flow and hence will modify the flamelet strain rate which is one of the major parameters in flamelet models. It is also clear that all issues cited above might not be completely treated in the limited time devoted to this study.

4. Program

This work will be done starting with the code developed by Dr. S. K. Lele at NASA Ames. This code is fully compressible and it will be modified and used in two different versions:

- Version 1 will have essentially the same base than the original code, will deal only with non-reacting flows, and will specifically address the effects of acoustic waves on vortex shedding and growth. It will also be used for the implementation of new boundary conditions and excitation methods adapted to acoustic treatments and different validation tests.

- Version 2 will have chemical reactions. This will require different modifications of the code and also some basic validation tests such as computation of laminar flames.

These two versions will be developed and used together. Since September 1st., Version 1 has been modified to provide easy pre- and postprocessing and is presently used to test the code performances on acoustic waves computations and implement more complex boundary conditions. Version 2 is being modified at the same time but will not be used before first validation tests of Version 1 will be finished.

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