The combustion program at CTR

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1. Introduction

Understanding and modeling of turbulent combustion are key problems in the computation of numerous practical systems. Because of the lack of analytical theories in this field and of the difficulty of performing precise experiments, direct numerical simulation (DNS) appears to be one of the most attractive tools to use in addressing this problem. The general objective of DNS of reacting flows is to improve our knowledge of turbulent combustion but also to use this information for turbulent combustion models. For the foreseeable future, numerical simulation of the full three–dimensional governing partial differential equations with variable density and transport properties as well as complex chemistry will remain intractable; thus, various levels of simplification will remain necessary. On one hand, the requirement to simplify is not necessarily a handicap: numerical simulations allow the researcher a degree of control in isolating specific physical phenomena that is inaccessible in experiments.

CTR has pursued an intensive research program in the field of DNS for turbulent reacting flows since 1987. DNS of reacting flows is quite different from DNS of non-reacting flows: without reaction, the equations to solve are clearly the five conservation equations of the Navier Stokes system for compressible situations (four for incompressible cases), and the limitation of the approach is the Reynolds number (or in other words the number of points in the computation). For reacting flows, the choice of the equations, the species (each species will require one additional conservation equation), the chemical scheme, and the configuration itself is more complex:

(1) The choice of the conservation equations to solve is open to discussion. Most DNS of non-reacting flows have been performed for incompressible constant-density flows. For reacting flows, incompressible (constant density, constant pressure), low-Mach number (variable density, constant pressure), or fully compressible formulations (variable density, variable pressure) may be used. Although incompressible formulations produce interesting information regarding certain mechanisms present in a turbulent flame, they are limited by the assumption of constant density and temperature ("cold" flames or zero heat release), which makes their results too different from real flames in many dynamical aspects. The following step for combustion is, therefore, to use a low-Mach number approximation where pressure is supposed to be constant but density may change because of heat release (Rutland 1989, Rutland and Trouve 1990, Mahalingam 1989). In

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this formulation, acoustic waves are eliminated and the time step is not limited by the classical Courant condition on sound speed, making the formulation especially well-suited to slow flows (low-Mach number). Finally, performing a fully compressible computation is also possible and has the advantage of offering an easier treatment of boundary conditions.

(2) The choice of the number of species to consider and of the chemical scheme is a source of controversy and speculation. Chemists argue that a realistic computation of most hydrocarbon fuels combustion requires at least thirty species while DNS specialists indicate that the numerical constraints of an unsteady computation in three dimensions make such a computation practically impossible today. In fact, the choice of the chemical scheme is essentially dependent on the question to address: studying the folding of premixed flames in low-intensity turbulence may be done without any chemistry at all (the knowledge of a flame speed is sufficient) while considering pollution problems with DNS will require a reasonably complete chemical scheme. The latter computation will be much more realistic (and expensive), but the former may also be quite valuable. Interesting results on turbulent combustion (Yeung *et al.* 1990, Cant and Rutland 1990) have been obtained with codes of the first type (where chemistry is absent).

(3) The choice of the configuration and of the corresponding boundary conditions leads to additional difficulties. Most DNS of cold flows are performed in periodic domains. Periodicity is not achieved in most reacting flows, and, therefore, one must specify new boundary conditions which are compatible with the precision of DNS and are able to treat inlet and outlet flows, for example. Coupling phenomena between inlets and outlets are quite common in DNS because the numerical schemes which are used have very low artificial viscosity. Therefore, all waves (especially numerical or unphysical waves) may travel on the grid and propagate from the outlet to the inlet (Buell and Huerre 1988, Poinsot and Lele 1992). For incompressible or low Mach number formulations (Rutland and Ferziger 1989, Lowery and Reynolds 1987), the specification of boundary conditions which prevent these phenomena requires a fine tuning to be compatible with the pressure solver used inside the domain. "Convective conditions" may be used near outlets to satisfy global mass conservation. Another solution is to sacrifice a certain part of the computational domain near the outlet and use it as a buffer zone where perturbations are damped by a high artificial viscosity before they reach the outlet (Rai and Moin 1991). There is a large body of literature on non-reflecting boundary conditions, and there is no doubt that it is one of the major problems in the development of DNS codes for reacting flows.

(4) Because of cost considerations, the possibility of performing two-dimensional computations is often used, and the merits of this approach versus three-dimensional cases remain to be determined. The problem is similar to the choice of a chemical scheme: first-order arguments such as "Turbulence is always three-dimensional" do not always lead to sound numerical approaches. The situation here is different from non-reacting cases where the structure of turbulence is (indeed) intrinsically three-dimensional. For premixed flames, DNS (Ashurst 1991, Cant and Rutland

1990) shows that the probability of finding a cylindrical (2D) flame sheet is much higher than the probability of finding a really 3D spherical flame shape. Two-dimensional flame geometries appear to be the usual rule in real flames even though the flow field ahead of these flames is fully three-dimensional. When one considers the prohibitive cost of three-space dimensional computations for reacting flows, two-dimensional simulations remain an interesting and fruitful approach, and the rule at CTR has been to use them as often as possible.

(5) To be complete, a DNS of reacting flows should also include a description of heat transfer (radiation and convection) because heat losses near flame fronts may be important when quenching phenomena are considered.

(6) The choice of a numerical algorithm is strongly dependent on the assumptions used for the computation. In the case of constant density ("cold") flames, the codes used are the classical incompressible DNS codes for cold flows which are mostly based on spectral methods. The accuracy of these methods is well known as well as is their major drawback: the difficulty of using boundary conditions which are not periodic. Because of this difficulty, recent DNS work has used high-order finite difference schemes (Lele 1992) or mixed schemes which use spectral methods in two directions and a finite difference method along the non periodic direction (Lowery and Reynolds 1987).

2. Achievements

Research at CTR has focused on all aspects of the problem indicated above. Different approaches have been used and the main accomplishments are summarized below:

- from CTR experience in DNS of 'cold' flows, specific numerical schemes were developed for reacting flows. These schemes use either spectral methods (Rutland and Trouve 1990) or compact Pade schemes (Lele 1992) to estimate spatial derivatives. Finite difference schemes have been the most widely used and are usually fourth- or sixth-order accurate in space. Explicit time-advancement is used (Runge Kutta). In most practical situations they offer a performance which is comparable to spectral methods while being much more adapted to the treatment of complex boundary conditions.

- a new technique to implement boundary conditions in DNS codes for reacting flows was developed from an initial idea valid for inviscid flows (Thompson 1987) and validated in many different situations (acoustic waves and vortices leaving the computation box, Poiseuille flow, reacting and non reacting shear layers, sub- and supersonic flow) (Poinsot and Lele 1992). The same method has been used in all CTR DNS codes for combustion since 1990. It appears that compressible formulations lead to easier treatments of boundaries than incompressible formulations because waves are explicitly computed and available for boundary conditions. (Unfortunately, this is achieved at a higher cost).

- two-dimensional computations were performed and provided many new insights into the physics of quenching in premixed turbulent flames (Poinsot *et al.* 1991)

and the dynamics of these flames (Haworth and Poinsot 1992). These works were based on flame–vortex interaction as well as on flame–turbulence interaction. Simple chemical models have been used ($Fresh \rightarrow Burnt$), but fully compressible approaches with variable density and large activation energies were utilized for these computations. Simple models for heat losses were used. These results have shown that some classical ideas in turbulent combustion theory were not justified: for example, small scales appear to be much less efficient than expected from classical analysis. These results have been confirmed later by experiments (Roberts and Driscoll 1991, Roberts *et al.* 1993). They have also shown the importance of thermodiffusive effects even in turbulent flames. The importance of this mechanism has been confirmed by other methods in separate works (Wu *et al.* 1991, Abdel-Gayed *et al.* 1984, Becker *et al.* 1990). Effects of flame curvature were studied and predicted by comparing a DNS with an experiment performed at Stanford and asymptotic analysis (Poinsot *et al.* 1992).

- turbulent combustion models have been derived by combining multifractal analysis and flame vortex interaction results (Meneveau and Poinsot 1991). These models have been implemented in aircraft and rocket engine computations (Candel *et al.* 1990(a), (b)) as well as in piston engine computations in collaboration with Institut Francais du Petrole (Boudier *et al.* 1992). In all cases, the integration of DNS-based sub-models leads to considerable improvement of the prediction capacities of these codes. In collaboration with Ecole Centrale Paris, a KPP (Kolmogorov, Petrovski, Piskunov) analysis (Hakberg and Gosman 1984, Fichot *et al.* 1993) was used to predict the turbulent flame speed of planar turbulent premixed flame. The performances of models derived from DNS were analyzed and compared with classical models (Duclos *et al.* 1993).
- ignition in turbulent premixed flames was also studied at CTR (Poinsot 1991), and an ignition model based on this work was implemented and validated in KIVA (Boudier *et al.* 1992).
- three-dimensional computations were also developed, first in the constant density case (Rutland and Trouve 1993, Rutland 1989) and later with variable density and heat release (Trouve and Poinsot 1993). These computations have confirmed many of the results obtained in two dimensions and brought a large number of intrinsically 3D results concerning, for example, flame shape statistics, orientation, and straining characteristics. More generally, they have been used in many turbulent combustion models (Bray 1990, Bray and Cant 1991, Kostiuk and Bray 1993). Different collaborations with combustion specialists (Prof. Cant, Dr. Ashurst, Dr. Hakberg) have taken place in the last three years to exploit these data bases. They were performed with simple chemical schemes ($Fresh \rightarrow Burnt$).
- two-dimensional computations of flame-wall interaction with simple chemistry have been performed, and models have been derived from DNS results and applied in piston engines models (Poinsot *et al.* 1993).
- the feasibility of two-dimensional computations with complex chemistry and precise transport models was demonstrated in 1992 by coupling the CTR DNS code

with the SANDIA softwares CHEMKIN (for chemistry) and TRANSPORT (for viscosity and diffusion coefficients). This code, developed at Ecole Centrale Paris and CERFACS, was tested at CTR during the 1992 Summer Program. It allows the simulation of turbulent flames with complex chemistry and was applied to the prediction of turbulent H2-O2 flames with a Warnatz scheme (9 species and 19 reactions) (Baum *et al.* 1993(a), (b), (c)).

- CTR has also investigated other ways to make progress in the field of turbulent combustion and developed a new experiment at Stanford University (Prof. Bowman) in the field of flame-vortex interaction. The capability of combining DNS and experiment offers CTR a powerful tool to deal with the problem. This project is presented by Dr. Mantel and Dr. Samaniego in the following reports.
- Although most of the CTR work has focused on premixed flames, diffusion flames have also been studied, both in the core program (Vervisch 1992) and during summer programs. Two- and three-dimensional simulations for turbulent diffusion flames have been performed and have allowed the structure analysis of these flames. The influence of the chemical scheme (one- versus two-step reactions) on quenching was studied in 1992 (Chen *et al.* 1992(a)) as well as the validity of flamelet assumptions (Chen *et al.* 1992(b), Mell 1990) and pdf models (Fox *et al.* 1992).
- CTR has also contributed to the development of DNS of reacting flows in other research centers by distributing its basic code (for simple chemistry). This code is now used at Univ. of Colorado (Boulder), Sandia, Univ. of Madison, Institut Francais du Petrole, Stanford Univ., Ecole Centrale Paris and CERFACS.

3. Future plans

Two main objectives will be pursued in 1994 at CTR in the field of combustion research:

(1) Develop and improve CTR models for turbulent combustion

(2) Improve data bases available at CTR to help outside researchers test their own models.

To reach these objectives, four parallel approaches will be used in 1994:

(1) Flame - vortex interaction:

Flame vortex interaction studies will be pursued, both on the numerical and on the experimental side. Multiple goals may be reached through this study: to understand the basic features of flame-vorticity interaction, study flame generated turbulence, create artificial turbulent flames by sending periodic arrays of vortices into a flame front, check the validity of DNS by comparing them with experiments, and use joint experimental and numerical tools to explore larger ranges of parameters. The report of Dr. J. M. Samaniego describes this work in more detail.

(2) Complete three-dimensional data bases:

The work of Dr. Trouvé on three-dimensional data bases for premixed turbulent flames with heat release has opened new perspectives in the field of turbulent combustion models. Many models have been compared to DNS data bases (Poinsot

et al. 1992, Cant and Rutland 1990, Trouve and Poinsot 1993) and the ensemble of data bases and post processing techniques which has been developed has to be extended and made available to the outside community. Dr. T. Mantel is working on this problem and a description of his work is given in this report.

(3) Flame wall interaction studies:

The interaction between a cold wall and a flame has numerous practical implications but is poorly modeled at the present time: one needs to model the effect of the wall on the flame (possible quenching) but also the effect of the flame on the wall (increased heat transfer). Both aspects may be attacked using DNS. The first one was treated at CTR in 1992 (Poinsot and Haworth 1992, Poinsot *et al.* 1993) in collaboration with Institut Francais du Petrole (where a model was used for piston engine cases). In 1994, the study of this problem will be continued by using a full 3D channel flow simulation at CTR to study flame dynamics near a wall with stationary turbulence. This work will be done in collaboration with CERFACS where a model for heat transfer will be developed.

4) Stabilization of diffusion flames:

In addition to research dealing with premixed combustion, efforts at CTR also include investigations concerning nonpremixed combustion. The long term goal of this work is to provide an understanding of diffusion flame characteristics which can be used in developing models for large eddy simulations. These fundamental aspects of diffusion flames include the ignition and stabilization processes, which will be investigated in simple geometries using direct numerical simulations. The ignition and stability characteristics will be evaluated under a variety of configurations: a laminar flame where the triple-flame structure can be investigated; a shear layer where the effect of the splitter plate wake on the flame properties can be determined; and in analogy with the premixed studies, the effect of vortices on the above configurations will also be studied in order to examine possible quenching events. These areas are currently being investigated by Dr. G. Ruetsch using one-step chemical models. If need be, implementation of multiple-step chemistry (Chen et al. 1992(b)) can be included.

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