1 Project description

Direct Numerical Simulation (DNS) is a powerful tool for the detailed study of combustion phenomena. It solves the system of governing equations with high spatial and temporal accuracy and can provide information that cannot be obtained by other means. Unfortunately, it also carries a very high computational cost. Efficient numerical algorithms and parallelization are essential for simulating complex phenomena or problems of practical interest. During the last few years, our two-dimensional DNS code was used to study phenomena of fundamental interest in combustion with detailed chemistry and transport properties. The same algorithms were implemented in a parallel, non-reactive, three dimensional code with efficient solvers and very good scalability on a number of parallel architectures. The extended code will be the main tool for the study of laminar and early turbulent combustion processes. It is also the basis for the implementation of Large Eddy Simulation (LES) approaches for the simulation of turbulent combustion. During the last year the code has been used to study instabilities of jet diffusion flames close to extinction. For reactant Lewis numbers sufficiently less than unity, 3-D simulations with single-step chemistry and simplified transport could capture the cellular flames observed experimentally at EPFL. To study the axisymmetric flame oscillations observed for reactant Lewis number equal or greater than one, the axisymmetric form of the conservation equations was implemented in the code. We are currently trying to identify the appropriate rate parameters of the single-step reaction to get close to the diffusion flame extinction. The code is further extended with the implementation of detailed chemistry and transport and a parallel stiff integrator for the efficient integration of the species and energy conservation equations.

2 Main results

2.1 Code development

Our simulation tool is based on the spectral element discretization of the partial differential equations describing the conservation equation of mass, momentum, species, and energy for three-dimensional chemically reacting system at the low Mach number limit. The spectral element method combines the flexibility of the finite element method to discretize complex geometries with the accuracy of spectral methods. Locally, the mesh is structured, with the data and geometry expressed as sums of N^{th}-order tensor product polynomials [4]. Globally, the mesh is an unstructured array of deformed hexahedral elements. Temporal discretization is based on a high-order, operator-splitting formulation for low speed compressible reacting flow that permits large time steps. More information about the numerical algorithm can be found in [1, 2, 3, 4].

In collaboration with Dr. Paul Fischer (Argonne National Laboratories), we implemented the algorithms for reactive flow species and energy equations in a parallel, non-reactive, three dimensional, spectral element base code. The code uses scalable domain-decomposition-based iterative solvers with efficient preconditioners. The parallel implementation is based on the standard message-passing Single Program Multiple Data (SPMD) mode, where contiguous groups of elements are distributed to processors and the computation proceeds in a loosely synchronous manner; communication is based on the MPI standard. The code exhibits very good parallel efficiency and scalability properties, sustaining high MFLOPS, on a number of distributed-memory platforms. Currently, single-step chemistry and simple transport have been implemented. The code was used on the LAV 64-CPU Linux cluster for the simulation of jet diffusion flame instabilities close to extinction observed experimentally at EPFL.

During the last year we continued both code development and applications. In terms of further code development:

- The axisymmetric form of the conservation equations was implemented and validated. The reduction in problem size will allow us to more effectively study problems like the axisymmetric pulsating instabilies of jet diffusion flames.

- The code is enhanced with detailed chemistry and transport and a parallel stiff integrator. The general-purpose PVODE [5] integrator has already been coupled with the code and validated against already available results with single-step kinetics. Detailed chemistry and transport are currently implemented via coupling with the CHEMKIN package. This development will enable the direct numerical simulation of combustion phenomena in the laminar and the early turbulent regime.

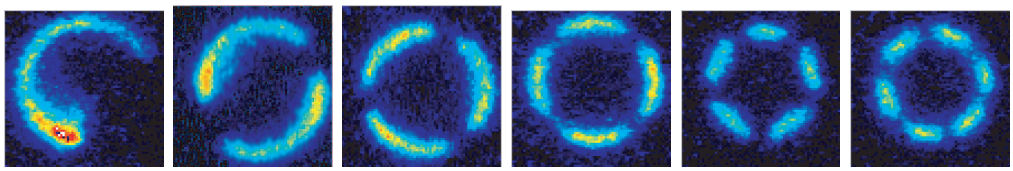
Turbulent reactive flows will be addressed with Large Eddy Simulations. In a parallel project, the code is used as the basis for the implementation of the Approximate Deconvolution Method (ADM) [6].

2.2 Applications

The code was used to simulate for the first time cellular diffusion flames. These have been observed experimentally at EPFL for jet diffusion flames close to extinction when the reactant Lewis number is sufficiently lower than one. The results were presented in the 30^{th} Combustion Symposium and will appear in the Proceedings of the Combustion Institute.

The EPLF free jet apparatus, consists of a contoured axisymmetric contraction with an area ratio of 100:1. The circular fuel nozzle of diameter $D = 0.75$ cm is surrounded by a a porous plate of 7.5 cm diameter, where the oxidizer mixture is introduced. A systematic experimental investigation of cell formation

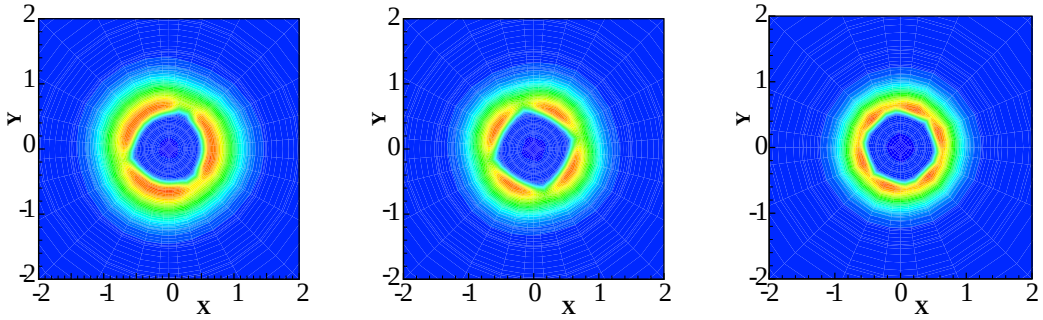
in CO_2-diluted H_2-O_2 circular jet non-premixed flames was performed on this burner and the observed cellular flames can be seen in figure 1.



(a) 1R-cell (b) 2R-cell (c) 3R-cell (d) 4S-cell (e) 5S-cell (f) 6S-cell

Figure 1: Streamwise integrated chemiluminescence images of CO_2-diluted H_2 and in CO_2-diluted O_2 coflow jet flames. Images are taken downstream from the jet axis. "R" designates rotating and "S" stationary cell patterns.

Three-dimensional simulations of the experimental setup were performed using single-step chemistry $2H_2+O_2 \rightarrow H_2$, with reaction rate $r = A\ T^n\ \exp(-T_a/T)\ [H_2]^2\ [O_2]$ and rate parameters $n = 0.91$, T_a=27.7 , and dimensionless heat of reaction ΔH_r=44.12. Constant but unequal Lewis numbers were used. Two resolutions were employed with 1166 and 2376 spectral elements with interpolating polynomial orders $6 \leq N \leq 8$ and $N = 4$ in each of the three spatial directions, respectively. The largest simulation had a total of about 600,000 points, corresponding to more than five million unknowns. By varying the dimensionless pre-exponential factor, A, the simulations captured the experimentally observed phenomena: existence of cellular structures with different number of cells close to extinction, co-existence of different cellular structures close to extinction (fig. 2), and sensitivity to noise, which can result in transitions from one cellular structure to another. More details can be found in the attached paper that will appear in the Proceedings of the Combustion Institute.



(a) (b) (c)

Figure 2: Temperature iso-contours of the (a) 3- ($A = 1.8 \cdot 10^8$, at z=0.8*D), (b) 4- ($A = 1.8 \cdot 10^8$, at z=0.8*D), and (c) 6-cell flame ($A = 2.5 \cdot 10^8$, at z=0.5*D)

We are currently studying axisymmetric pulsating instabilities that were also observed at EPFL when the fuel Lewis number is equal or larger than one. Diffusion flame instabilities depend significantly on a large number of parameters (initial mixture strength, Lewis numbers, proximity to extinction). Consequently, both experimental and numerical information are required to elucidate the underlying physics.

3 National collaborations

In collaboration with the Fluid Mechanics Laboratory of EPFL (group of Prof. P. Monkewitz), we are studying diffusion flame instabilities close to extinction. The work is a combination of experiments, numerical simulation and stability analysis.

Recently, we have started a collaboration with Prof. Patrick Jenny of the Institute of Fluid Mechanics at ETHZ. The aim is to perform direct numerical simulation of turbulent mixing under non-reactive and reactive conditions in order to obtain data for the development and validation of turbulent mixing models.

4 International collaborations

The parallel, three-dimensional reactive flow DNS code is being developed in collaboration with Dr. Paul Fischer of Argonne National Laboratory, USA.

In the framework of the simulation of diffusion flame instabilities, we are working together with Prof. Paul Papas of the Colorado School of Mines.

5 Conclusions and outlook

During 2004 we implemented and validated the axisymmetric form of the conservation equations, coupled the code with the general-purpose parallel stiff integrator PVODE, and started the implementation of detailed chemistry and transport using the CHEMKIN package. The linear scalability of our reacting flow code enabled the first simulation of cellular jet diffusion flames in the full three-dimensional context. We have also started the simulation of axisymmetric pulsations, another type of instability that has been observed in the same system.

In 2005, we plan to finish with the implementation of detailed chemistry and transport. The extended code will be used for the quantitative simulation of cellular flame instabilities. We will also continue the study of axisymmetric pulsations with single-step chemistry. In addition, we will perform direct numerical simulation of turbulent mixing under reactive and non-reactive conditions. The data will be used for the development and validation of turbulent mixing models.

6 Publications

C.E. Frouzakis, A.G. Tomboulides, P. Papas, P.F. Fischer, R.M. Rais, P. Monkewitz, and K. Boulouchos, "Three-dimensional numerical simulations of cellular jet diffusion flames", *Proc. Comb. Inst.*, **30**, (in press).

The publication is appended at the end of the report.

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