Three-Dimensional Detailed Simulation of Laminar Burners on Parallel Computers

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Abstract

Laminar flows involving chemical reactions play an important role in many practical applications. In this work a three-dimensional simulation dedicated to solving the Navier-Stokes equations in the low-Mach number limit is presented, using detailed chemistry and detailed transport. A complex three-dimensional configuration of a laminar methane/air burner is considered. Thanks to efficient numerical methods, accurate solutions can be obtained on such complex systems for acceptable computing times.

Introduction

It will be shown that it is possible using Computational Fluid Dynamics (CFD) to solve within a reasonable computing time complex problems involving coupled fluid flow, heat transfer and chemical reactions, even for configurations close to practical ones. In the present work laminar flows are considered, since they correspond to real engineering problems, for example domestic burners. A laminar gas flame is thus considered, as found in practice in such low-power domestic boilers.

Since most existing practical applications take place in the turbulent regime, there has been comparatively little work up to now concerning the accurate simulation of laminar reacting flows. The situation is very different for turbulent combustion, where a considerable quantity of reference information can be found (see for example [1–3]).

For laminar combustion using detailed chemistry and transport models, most publications are restrained to very simple, academic configurations. This is typically the case for (mostly one-dimensional) codes solving laminar flame structures, like for example propagating one-dimensional premixed flames (PREMIX [4]), propagating flames in flat channels [5], or counter-flow flames [6–8]. These codes are frequently found in research laboratories and play a very important role for basic research. But they cannot handle practical systems, since they are limited to one-dimensional problems or, for the most complex codes, to two-dimensional cases with elementary geometries.

A small number of more advanced simulation tools have still been developed. For example simulations using detailed reaction schemes in two-dimensional geometries have been employed to simulate ignition processes [9] or axisymmetric diffusion flames [10], both for simple fuels. Similar studies have been later on devoted to methane

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Proceedings of the European Combustion Meeting 2009

combustion [11,12], leading to a considerable increase in computing times. More recently detailed numerical simulations have been in particular published for axisymmetric methane Bunsen flames [13,14], sometimes associated to extensive comparisons with experimental results [14]. Further recent publications have been devoted to partially-premixed combustion [15–17]. These last publications and the follow-up works are probably the most elaborate ones describing a detailed validation procedure for laminar flames.

For all these results, the geometrical configuration has been limited to two dimensions (either planar or axisymmetric) and kept simple. Some attempts have also been reported to compute laminar hydrogen flames in elementary three-dimensional configurations [18], and more recently methane flames in two dimensions for more complex geometries [19–21], paying in particular attention to issues concerning grid resolution and parallel efficiency. But, to our knowledge, no three-dimensional laminar reacting flows associated with a more complex geometry have been investigated using detailed chemistry and transport models yet, leading to publication in international journals.

The present work describes our most recent efforts toward three-dimensional simulations using complete reaction schemes. In order to reduce the resulting computing times, these simulations rely on parallel computers. The investigated configuration corresponds to a household burner, shown in Figure 1. The diameter of the injection hole is 1.9 mm, the height of the inlet tubes is 6.3 mm. The full size of the the computational domain considered in the simulation is 2.5 × 2.5 × 25.1 mm.

Governing equations

Laminar flows involving chemical reactions are considered in this paper. In the presented application Mach numbers M are very low. It is observed that pressure variations through laminar flames at low Mach numbers are always of the order of magnitude of a few Pascal and stem mainly from hydrodynamical and not from compressibility effects. Stated differently, density variations only result from heat release due to chemical reactions and from changes in the mixture composition, but not from local fluid compression. Temperature and density vary in opposite directions, such that their effects within the ideal gas law compensate. These physical observations motivate the decomposition of pressure into a bulk background uniform thermodynamic pressure p_u and a hydrodynamic fluctuation term $\tilde{p}$ [22,23]:

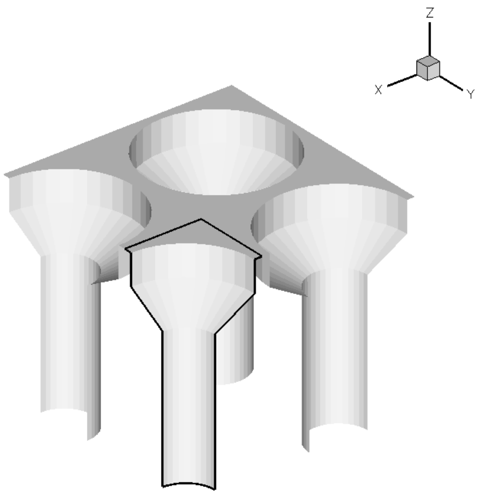

Fig. 1. General configuration of the investigated laminar burner. A methane/air mixture enters through the injection holes. Due to symmetry only the highlighted part (black edges) must be simulated.

$$p\left(\boldsymbol{x},t\right) = p_u\left(t\right) + \tilde{p}\left(\boldsymbol{x},t\right) \quad . \tag{1}$$

For the presented application (a domestic gas burner), the numerical domain is considered to be open, hence p_u equals the atmospheric pressure and is constant. If acoustic waves may propagate in the gas mixture, then an additional acoustic pressure term has to be considered. Since we do not address cases of acoustic/flame interactions here, we assume from now on that acoustic waves are either inexistent or of negligible effect on the flame structure and on the flow. Readers particularly interested in flame/acoustic interactions may, e.g., refer to [24,25] for specific details.

Within the low-Mach number approximation, the density appears as a function of temperature

T and mean molar weight W. When the numerical domain is opened to the atmosphere the influence of the hydrodynamic pressure $\tilde{p}$ on the density must be neglected. The full problem is then described by the following set of balance equations, written in conservative form for mass, momentum, mass fractions and enthalpy, solved in the present case:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \tag{2}$$

$$\begin{aligned}\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v v) &= -\nabla \tilde{p} \\ &+ \nabla \cdot \left\{ \mu \left(\nabla v + (\nabla v)^T \right) \right\}\end{aligned} \tag{3}$$

$$\begin{aligned}\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho Y_k v) &= -\nabla \cdot (\rho Y_k V_k) \\ &+ W_k \dot{\omega}_k \ , \quad 1 \le k \le K-1\end{aligned} \tag{4}$$

$$\begin{aligned}\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho h v) &= \\ &\nabla \cdot \left(\lambda \nabla T - \rho \sum_{k=1}^{K} h_k Y_k V_k \right)\end{aligned} \tag{5}$$

Using a unity Lewis number assumption for the diffusion model, equations (4) and (5) become much simpler:

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho Y_k v) = \nabla \cdot \left(\frac{\lambda}{c_p} \nabla Y_k \right) + W_k \dot{\omega}_k \tag{6}$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho h v) = \nabla \cdot \left(\frac{\lambda}{c_p} \nabla h \right) \tag{7}$$

Equation (6) is solved for $K-1$ species, because the last species (the nitrogen) is a dilutant, determined using: $Y_{N_2} = 1 - \sum_{k=1}^{K-1} Y_k$.

A stoichiometric premixed methane/air flame at the inlet, atmospheric pressure at the outlet and fresh gas temperature of 298 K is considered in these computations. The complete set of chemical species and elementary reactions, with their Arrhenius coefficients A_i (pre-exponential factor), β_i (temperature exponent) and E_i (activation energy), is taken for methane/air flames from [26]. This detailed reaction scheme involve 29 species and 141 elementary reactions. The injection conditions correspond to a mixture of methane and air with $Y_{CH_4} = 0.0551$, $Y_{O_2} = 0.22$, $v_{\text{inlet}} = 0.653$ m/s and $T = 298$ K at the inlet. A constant temperature of 298 K is assumed on the inlet walls.

Numerical solution

The simulation of a three-dimensional laminar methane/air burner using detailed chemistry and detailed transport model is now considered [27]. Using this description for three-dimensional configurations on a growing number of grid elements rapidly leads to a large discretized equation system, to a tremendous computation time and to a huge memory requirement. In this case parallel computations are absolutely necessary.

The numerical simulation is performed using the in-house code *UGC*$^+$, developped in collaboration with the University of Heidelberg (IWR, G. Wittum). This code has been optimized for the computation of steady laminar low-Mach number flows with chemical reactions [28,29]. It is designed as an application of the multi-purpose *UG*-library [30]. *UG* is a modular numerical toolbox originally aimed at investigations of multigrid methods on various model problems described by sets of partial differential equations.

UGC$^+$ is based on two main modules: a low-Mach Navier-Stokes solver and a thermo-reactive solver. A joint module has been developed to achieve the full coupling of the two sub-modules into one single system of Partial Differential Equations. The two solvers are in charge of their own diagonal block of the Jacobian matrix and there is an information interchange between them (mass fluxes, density and viscosity). Off-diagonal blocks of the Jacobian matrix are simply evaluated by numerical differences.

The discretization in space is based on a Finite Volume approach, using the solution first proposed by Schneider and Raw [31] and further developed by Nägele [32]. The method is based on a collocated grid, where the control volume boxes are formed by a dual grid, as shown in [33].

Fluxes are evaluated at the integration points on the basis of the local ansatz functions on the elements. The non-linear terms are upwinded with the skewed upwind method proposed in [34].

Parallel issues

The *UGC*$^+$ code attempts to find steady solutions through time-marching. Time discretization is of first-order implicit type. The value of the time-step can be adapted at each iteration, according to convergence or any user-defined condition. The unsteady equations are solved by fixed-point or approximate-Newton iterations and the user can freely specify how often the Jacobian matrix has to be assembled. The linearized equations are then solved by a Bi-CGSTAB algorithm, preconditioned by multigrid V-cycles with an ILU smoother. An adaptive grid is used to increase resolution for such multi-scale problems (thin reaction zones, large geometries).

The *UG* library is built on top of the parallel module DDD [35], employed for efficient migration on parallel supercomputers. Most of the parallel programming issues, in particular data integrity and communication, are done within DDD modules, which are completely independent of the application. It runs on shared as well as distributed memory machines or a combination of them, a technology quite often used in modern supercomputers.

An adaptive grid is used to increase spatial resolution. Adaptive grid refinement is done a posteriori with an indicator based on the actual solution. Here, the mass fraction of the radical HCO, a very good tracer of the reaction front, is used to define elements on the grid to be refined or coarsened. Hence, the resolution and numerical discretization errors are reduced, since areas with higher gradients are better discretised, leading to less numerical diffusion.

For load-balancing purposes the CHACO library is coupled with *UGC*$^+$, and provides different load-balancing strategies. In the present case the RCB (Recursive Coordinate Bifurcation) algorithm is applied. RCB was first proposed as a static load-balancing algorithm in [36], but is also attractive as a dynamic load-balancing algorithm, as demonstrated for the present case. In RCB, the computational domain is first divided into two regions by a cutting plane orthogonal to one of the coordinate axes so that half the work-load is in each of the sub-regions.

Computational grid

The smallest grid spacing obtained in the present computations is 20 μm in the $x - y$ plane and 40 μm in the z-direction. The initial grid contains 4 330 hexahedral finite-volume cells. This relatively large number of cells is needed to describe the geometry in an accurate manner and to preserve the structural details, especially for the faces with complex geometry. The worst skewness parameter in the initial grid is 0.7, indicating that the hexahedral elements are only slightly distorted in the worst region. During the computations the numerical grid contains between 200 000 and 270 000 finite-volume cells after reaching the third level of grid refinement. The computation on the refined grid with detailed chemistry produces a very large algebraic system and thus requires a huge amount of computer memory.

Results and Discussion

All the simulations have been carried out on the Kármán cluster in Magdeburg equipped with 68 dual-nodes (2.1GHz AMD Opteron quad-processors). In this study, altogether 320 cores using a high-speed Infiniband interconnection have been employed to perform these detailed computations, involving 29 species equations on almost 300 000 grid elements.

The computed temperature in the full domain is shown in Figure 2, revealing the very complex, three-dimensional structure of the flame. Visualization relies on the software Tecplot, but compatibility issues with the refined grid employed by *UGC*$^+$ often limit the quality of the resulting images, leading to graphical artefacts.

The mass fraction of the HCO distribution can be seen in Figure 3. This very reactive intermediate species can be seen as a marker of the flame front.

Here again, the three-dimensional structure of the flame appears clearly.

Figure 4 represents the mass fraction of CO, one of the major pollutant species in methane combustion.

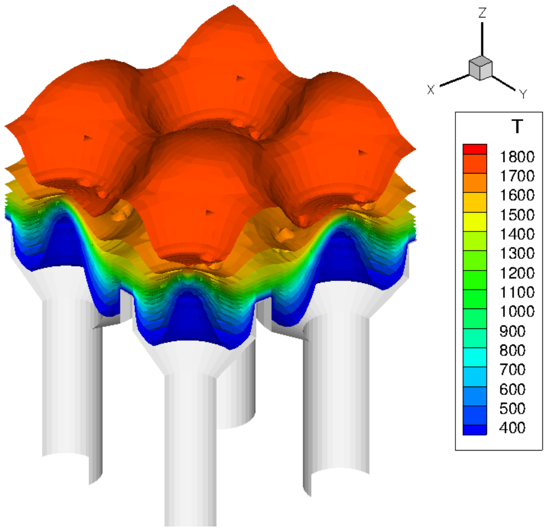

Fig. 2. Temperature distribution in the investigated domain.

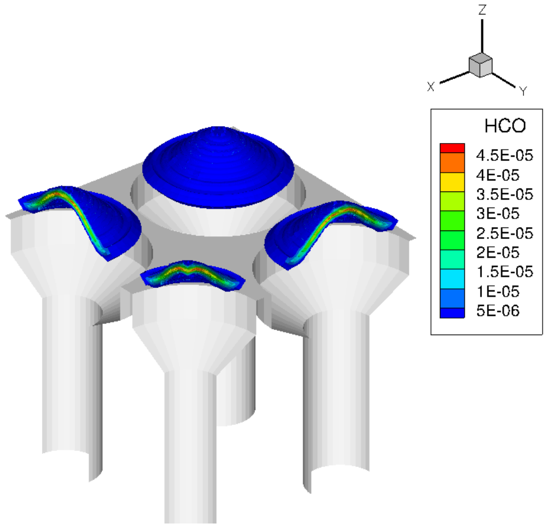

Fig. 3. Mass fraction of the HCO radical in the investigated domain.

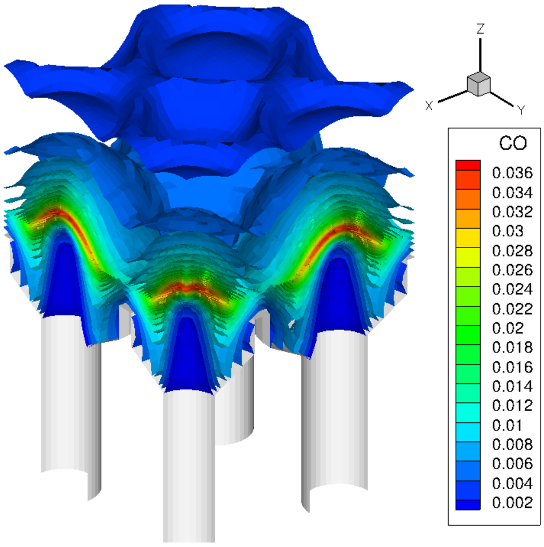

Fig. 4. Mass fraction of the CO pollutant species in the investigated domain.

Conclusions

We have demonstrated in this study that the simulation of complex flows involving heat transfer and chemical reactions is possible, provided very efficient numerical methods are used for the CFD procedure (here the in-house UGC+ code). In this case, optimal solutions can be obtained with a small number of iterations and acceptable computing times. Further investigations are presently conducted to decrease even more the needed computing time and therefore have access to even more realistic, three-dimensional configurations, described with more refined models using a higher number of input parameters.

Acknowledgements

The development of the program UGC^{+} would not have been possible without the Ph.D. work of S. Paxion and R. Baron.

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