Numerical Simulations of Supersonic Combustion of Methane-Hydrogen Fuel in an Experimental Combustion Chamber

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An accurate CFD modeling requires a big computational time, which can be significantly reduced by using parallel processing. A great progress in performance of computers on PC platform and fast networks permits creating powerful computational systems with distributed memory (DM). Such systems can compete with supercomputers being much cheaper and easier for maintenance.

The research federation EPEE[1] (Energétique, Propulsion, Espace, Environnement) has provided for its members, laboratories of the CNRS and University of Orléans, a PC cluster operating under the LINUX system. The PC cluster includes 24 bi-processor nodes (AMD Athlon 1.2 GHz, FSB 266 MHz) connected to a master node. Eight nodes are linked by Myrinet ultra-fast network and others by Fast Ethernet network. This configuration makes the system available for solving computational tasks with different requirements for the frequency of the data exchange between parallel processes.

MBDA-France, ONERA, and CNRS-LCSR (Laboratory of Combustion and Reacting Systems) collaborate on the development and implementation of numerical models for CFD applications in combustion. CNRS-LCSR has recently obtained a parallelized version of the MSD code and have installed it on the PC cluster of the EPEE. MSD is a CFD code developed by ONERA for scientific and industrial applications in aerodynamics and propulsion. The code integrates a number of turbulence models and several turbulent combustion models[2]. ONERA and MBDA-France extensively use the MSD code in the scope of their hypersonic projects. The MSD code can treat multidimensional complex configurations with a multidomain structure. Domains are processed independently with periodic updating of boundary conditions or overlapped zones. This kind of processing is especially advantageous for DM parallel systems. A computational job can be optimized in terms of the domain number and domain sizes. The parallelized version of the MSD code uses MPI instructions providing management of parallel computation processes.

Among CFD problems, simulations of hydrocarbon combustion are especially resource consuming when they involve detailed chemical models. Hydrocarbon fuels, being the most important combustibles, feature very complex oxidation chemistry even if they are as simple as methane or ethane. Thus the choice of an appropriate chemical model offers a difficult tradeoff problem.

A reduced kinetic mechanism recently developed at CNRS-LCSR for methane-hydrogen fuel comprises 79 reactions between 21 species among which 16 species must be included in transport equations, others are assumed in a quasi-steady state and their concentrations are evaluated from explicit algebraic relations. Simple reactor models SENKIN and PSR from the CHEMKIN-II program package were used for extensive tests of the mechanism under conditions of the shock-tube and perfectly stirred reactor. The reduced mechanism, validated against its parent comprehensive mechanism[3] and available empirical correlations, has demonstrated accurate predictions of the ignition delay, extinction limits, and temperature profiles within a large domain of mixture parameters (equivalence ratio, initial temperature, hydrogen mass

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fraction). The reduced mechanism has been implemented into the MSD code; thus it is actually available for multidimensional combustion modeling.

Numerical simulations of a reacting methane-hydrogen supersonic jet in a duct have been performed to assess the MSD performance on the parallel PC platform. The configuration of the duct corresponds to that of the LAERTE facility at ONERA. The LAERTE test facility has been created to investigate fundamental features of supersonic diffusion combustion[4]. Up to date, several experimental studies of the hydrogen combustion resulted in a detailed set of experimental data thus providing a base for CFD tools validation[2]. Combustion experiments with methane-hydrogen mixture are anticipated in a near future.

Schematic view of the LAERTE combustion chamber is given in Fig. 1. It has a 2-D main nozzle with a square cross-section at the exit of 45×45 mm^2. Coaxial axisymmetric nozzle with an exit diameter of 6 mm creates a fuel jet. Both nozzles are designed for an exit Mach number of 2. The total length of the supersonic duct is equal to 870 mm and the central nozzle is projected into the duct by 33 mm. The supersonic duct consists of a constant area portion 370 mm long and a constant width divergent portion with a half angle of 1.15º. A hydrogen-fueled flame heater supplies the main oxidizer flow to the combustion chamber.

The combustion simulations have been made using a purely implicit time-marching scheme to obtain a steady state solution. Numerical fluxes are approximated by a second-order MUSCLE scheme, which is based on the Roe-type averaging. Turbulence transport terms are calculated according to the standard k-ε model. For the sake of simplicity, an equivalent axisymmetric configuration of the computational domain has been accepted instead of the real 3-D shape.

The following conditions have been selected for the simulations: Mach number of the oxidizer and fuel flows of 2, static pressure at the duct entrance of 0.8 bar, total temperature of the oxidizer flow of 1850 K, total temperature of the fuel flow of 300 K. The oxidizer composition corresponds to the vitiated air coming from the flame heater.

Results corresponding to the pure hydrogen injection are presented in Fig. 2. Colored zones in the background show the static temperature field and the dashed contours trace constant levels of the local equivalence ratio (ER). The flow remains supersonic excepting a region around the axis in the middle of the duct. The jet core is about 0.1 m long, nevertheless the mixing process is rather slow because the stoichiometric surface is always far from the axis, and the central zone is occupied by a very rich mixture (ER > 4). The ignition takes place at 60-70 mm from the central nozzle in a lean zone, where the temperature is higher. On the lean side of the mixing layer, the flame boundary occurs at low ER levels, close to 0.1. On the rich side, the oxidizer penetrates to the axis but it is consumed while T rises up to 1000 K, and O_2 disappears at ER = 10.

A comparison between the computational and experimental results is given in Fig. 3, which shows wall pressure profiles. In spite of some simplifying assumptions, the computed pressure profiles are in a fairly good agreement with the experimental data.

Under the given test conditions, the self-ignition of methane cannot be obtained because of too big induction time. Addition of some hydrogen can significantly accelerate the ignition process. By varying the mass fraction of H_2 in the fuel, it has been found that the combustion is attainable at a H_2 mass fraction of 20%. This case is illustrated in Fig. 4 in the same manner as in Fig. 2. The combustion zone has a form of acute wedge starting approximately at 0.4 m from the injection section. The Mach number varies between 1.2 and 1.4 in this region. From a close examination of parameter profiles, it can be noted that ignition effects occur at 0.3 m from the injector causing a local maximum on the cross-sectional profile of T.

An interesting finding has been made from the analysis of concentration profiles in the mixing layer. Oxygen penetrates to the central zone of the jet before the ignition and is consumed close the combustion zone. While CH_4 is decomposed and partially oxidized, the relative mass fraction of H_2 increases reaching 50% when the conversion of CH_4 is amounted to 75%. A similar behavior is observed close to the ignition point in a fuel-lean zone. This means

that the presence of H_2 considerably accelerates all phases of the CH_4 conversion. Being in comparable molar proportion with H_2, CH_4 appears to be more important consumer of active particles.

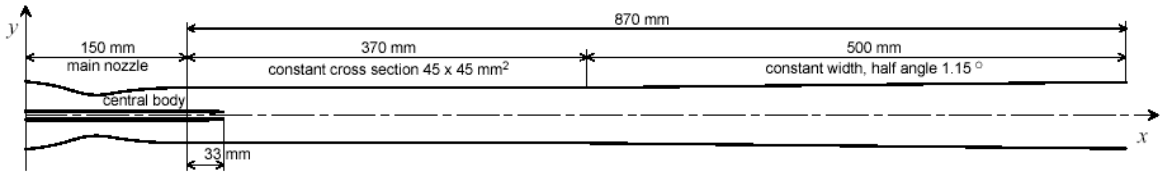

Fig. 1. Geometry of the LAERTE combustion chamber

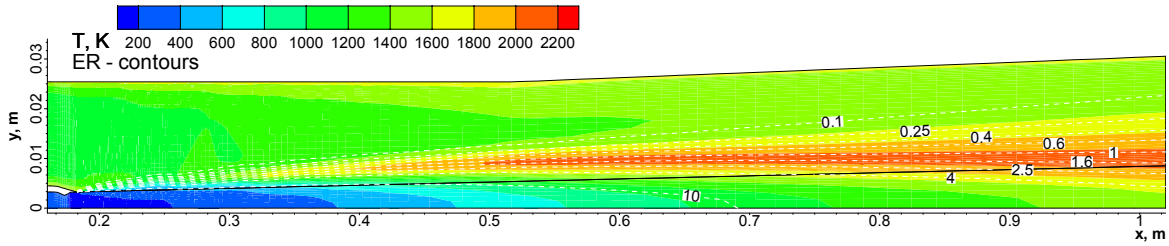

Fig. 2. Hydrogen combustion: Temperature and ER fields

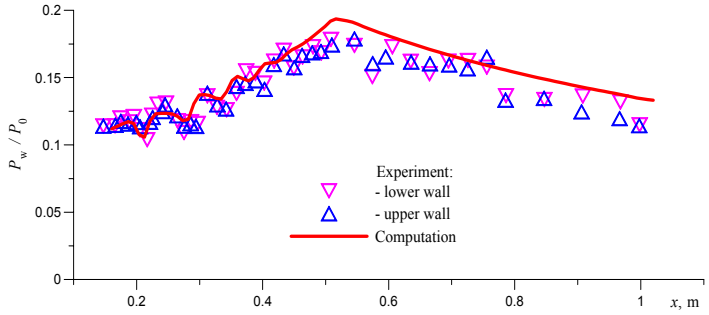

Fig. 3. Hydrogen combustion: Measured and computed wall pressure

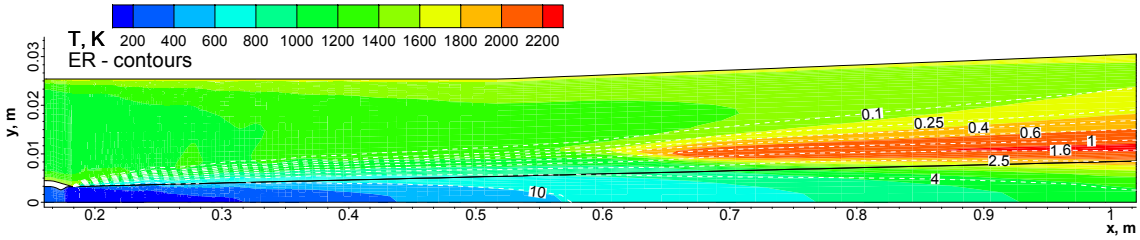

Fig. 4. Methane-hydrogen combustion: Temperature and ER fields

Acknowledgements

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