Large Eddy Simulation of an ultra-micro combustion chamber

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Abstract - The goal of this paper is to investigate the performance of microcombustors. Such field is currently under rapid development in particular for propulsion, e.g., for UAVs, and micro-electrical power generators. This study is focused on a cylindrical microcombustor fed by methane and air, with diameter and height 0.025m and 0.06m, respectively. A 3D LES is performed, using the Flamelet model for the combustion and the detailed GRIMech 3.0 mechanism for the chemistry. A preliminary series of non-reacting numerical simulations were necessary to identify the correct methane inlet duct diameter that avoids “reverse ingestion” (air entering the methane duct and premixing with the fuel upstream of the injection point). The maximum temperature inside the chamber, the gas exhaust temperature and pressure and the wall heat flux are reported and discussed. Combustion efficiency is analyzed from an entropy viewpoint. This work is a contribution to a better understanding of the most convenient design guidelines for future microcombustor applications, and to a more accurate estimate of the performance parameters to apply to first-order design.

1. Introduction

An investigation of the performance of a microcombustor for possible use in ultra-microturbines and micropropulsion is presented in this paper. The field of ultra-micro thermo-electric/electronic devices is rapidly developing under the pressure of new and more stringent requirements posed by the increasing need for portable power generation. In particular, three main areas of interest for ultra-micro-combustion exist: propulsion, UAV (“drones”) for tactical and meteorological recognissance, and portable electrical power generation.

The analysis was aimed at the detection and quantification of scale effects and was performed by means of a 3D unsteady LES of the combustion of a methane/air mixture in a cylindrical Chamber that provides almost 2KW of thermal power.

In this work the “dynamic kinetic energy subgrid model (DKE)” (Kim and Menon, 1997; Kim, 2004) is used. Contrary to the usual subgrid scales models (classic (Smagorinsky, 1963) or dynamic (Lilly, 1992; Germano, 1996) Smagorinsky-Lilly-type models) that assume the existence of a local equilibrium range between the transferred energy through the grid-filter scales and the dissipation of kinetic energy at the subgrid scales, the DKE model solves an additional subgrid kinetic energy transport equation. The model is thus more accurate but it requires higher computational effort (it solves one more equation); however, in the highly stretched flow studied here, where the (swirling) mean streamlines curvature is very high, of the order of 0.001m and smaller, this extra CPU cost brings sufficient benefits to warrant its adoption.

To improve the near-wall accuracy, an enhanced wall treatment is used (Werner and Wengle, 1991); here too, the strong curvature demands higher accuracy in the wall velocity resolution than a classical law of the wall.
In the first simulations, it was found that the kinetic energy of the inlet air jet was high enough to cause air ingestion into the methane duct: since a pre-mixing would be potentially damaging due to the unavoidable high thermal flux in the last portion of the methane injection tube, a preliminary non-reacting analysis was performed to identify the largest, ingestion-free methane duct diameter (for a fixed fuel mass flow rate). The final design has been modified accordingly, and has a methane duct of 0.0015m (less than a half of the initial design datum of 0.004m).

The reacting simulation has been carried out on this ingestion-free geometry: the “combustion coupling” is modeled by “67 flamelets” (Dixon-Lewis, 1990; Bray and Peters, 1994; Kim and Williams, 1997; Peters, 1984; Peters, 1986; Pitsch and Peters, 1998; Pitsch et al., 1996; Sivathanau and Faeth, 1990) while the chemistry is reproduced by a detailed mechanism (GRIMech3.0, 1994) defined by 53 species and 325 reactions, using Arrhenius relations.

Temperature maps, wall heat fluxes and an entropy-based combustion efficiency are the most important results provided.

This paper is structured as follows: Section 2 describes the domain geometry and the specified operating conditions; Section 3 contains a brief discussion of the turbulence models adopted, and Section 4 presents and discusses the results.

This work is part of a wider work that comprises experimental analysis too, which will be reported and compared in the future for a deeper understanding of combustion phenomena in microcombustion chambers.

2. Combustion Chamber and Operating Conditions

The combustion chamber geometry and dimensions influence the mixing dynamics, and consequently the combustion efficiency, due to the strong effects of the aspect ratio (D/L) on the mean streamline curvature and on the swirling motions.

Especially for the intrinsically low inlet Reynolds numbers typical of ultra-microdevices, there is the need to enhance the mixing of the air with the fuel immediately downstream of the fuel injection point, to facilitate fuel atomization and maximize access to oxygen: therefore, the air intake duct is tangential to the chamber and methane is injected in a direction perpendicular to the air mean flow (figure 1).

The diameter of the chamber is 0.025 m, its length 0.06 m (aspect ratio=0.416). The methane feeding duct has a diameter of 0.0015m, the air duct 0.005m. The exhaust duct on the upper side of the chamber has a diameter of 0.01m. Figure 1 shows the combustion chamber domain divided into slices for ease of visualization: the domain is discretized by 870000 unstructured cells, so that at the wall $y^+ \approx 5$ and $\Delta y^+ \approx 1$ in spite of the high stretching imposed by the elongated geometry.

Figure 1 refers to the final geometry: as mentioned in the Introduction, the original design was affected by air ingestion into the methane duct, and had to be properly modified. Figures 2 and 3 show the first trial geometry and the final design one; it is clear that the recirculation backflow air bubble inside the methane duct apparent in the first configuration is absent in the final one.

The two geometries differ for the methane/air the kinetic energy ratio, $M$, defined as:

$$M \equiv \frac{\rho_f v_f^2}{\rho_{\text{air}} v_{\text{air}}^2}$$
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Where “ox” stands for oxidant and “f” for fuel; $M$ is equal to 0.00105 and 0.038 in the first and final configuration respectively.

The final operating and boundary conditions are reported in Table 1; the fuel inlet Reynolds number is in the transitional regime, while the Re$_{air}$ is turbulent.

With this inlet conditions the dimensionless swirl number, $S$, defined as the axial flux of swirling momentum divided by the axial flux of axial momentum, times the equivalent nozzle radius is:

\[
S = \frac{\int \rho u_z u_r r dA}{r \int \rho u_r^2 dA} \approx 0.47
\]

This feature is characteristic (and peculiar) of microcombustors, thence the importance of an accurate analysis of the Reynolds maps inside the combustion chamber in order to identify and possibly locate laminar (or relaminarization) zones.

It is well known that the possibility of relaminarization is enhanced by combustion that causes an increase of the effective viscosity of the burning mixture; on the other hand, the slight expansion inside of the chamber introduces a contrasting effect, so that the final regime is determined by the imbalance and dynamic competition between these two effects.

![Figure 1: Representative geometry of the micro-combustion chamber](image)

Table 1: Operating Conditions

<table>
<thead>
<tr>
<th></th>
<th>Methane</th>
<th>Air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate [kg/s]</td>
<td>$3.93 \cdot 10^{-3}$</td>
<td>$1.9 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Inlet Temperature [K]</td>
<td>300</td>
<td>700</td>
</tr>
<tr>
<td>Outlet Pressure [atm]</td>
<td>2.</td>
<td>2</td>
</tr>
<tr>
<td>Inlet Velocity [m/s]</td>
<td>18</td>
<td>100</td>
</tr>
<tr>
<td>Inlet Viscosity</td>
<td>$2 \times 10^{-5}$</td>
<td>$3.29 \times 10^{-5}$</td>
</tr>
<tr>
<td>Re</td>
<td>2000</td>
<td>7500</td>
</tr>
<tr>
<td>Kinetic Energy Ratio, $M$</td>
<td></td>
<td>0.038</td>
</tr>
<tr>
<td>Global equivalence ratio</td>
<td></td>
<td>0.355</td>
</tr>
</tbody>
</table>
3. Turbulence, Combustion and Numerical Models

3.1 Large eddy simulation & the kinetic energy sub-grid scale model

The LES approach is used in this study to model turbulence. More precisely, the unknown sub-grid stresses resulting from the filtering operation are modeled by means of the “dynamic kinetic energy subgrid-scale model” (Kim and Menon, 1997).

This model accounts for the transport of the subgrid-scale turbulent kinetic energy: this means that the assumption of the existence of a dynamic equilibrium range between the energy transferred through the resolved scales and the dissipation of kinetic energy at small grid-scales (assumption common to all other subgrid algebraic models) is not used here, and an additional equation for the transport of subgrid kinetic energy is introduced to more accurately reproduce the relevant phenomenology.

This SGS turbulent kinetic energy transport model accounts for the history and non-local effects, having the potential to benefit complex flows with non-equilibrium turbulence.

The subgrid kinetic energy is defined by:

\[ k_{sgs} = \frac{1}{2} \left( \overline{u_i^2} - \overline{\tilde{u}_i^2} \right) \]  (3)

Which is obtained by contracting the subgrid-scale stress:

\[ \tau_{ij} = \rho \overline{u_i u_j} - \rho \overline{\tilde{u}_i \tilde{u}_j} \]  (4)

The subgrid-scale eddy viscosity, \( \mu_t \), is computed using \( k_{sgs} \) as:

\[ \mu_t = C_1 k_{sgs}^{1/2} \Delta_f \]  (5)

Where \( \Delta_f \) is the filter size computed from \( \Delta_f = \frac{V^{1/3}}{2} \).

The subgrid-scale stress can then be written as:
\[ \tau_{y} - \frac{2}{3} k_{sgs} \delta_{y} = -2C_{k} k_{sgs}^{3/2} \Delta_{f} \bar{S}_{y} \]  

(6)

Where \( \bar{S}_{y} \) is the rate of strain tensor for the resolved scale, defined by:

\[ \bar{S}_{y} = \frac{1}{2} \left( \frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}} \right) \]  

(7)

\( k_{sgs} \) is obtained by solving its modeled transport equation:

\[ \frac{\partial k_{sgs}}{\partial t} + \bar{u}_{j} \frac{\partial k_{sgs}}{\partial x_{j}} = -\tau_{ij} \frac{\partial \bar{u}_{i}}{\partial x_{j}} - C_{t} \frac{k_{sgs}^{3/2}}{\Delta_{f}} + \frac{\partial}{\partial x_{j}} \left( \frac{\mu_{t}}{\sigma_{k}} \frac{\partial k_{sgs}}{\partial x_{j}} \right) \]  

(8)

In the above equations, the constants \( C_{k} \) and \( C_{t} \) are determined dynamically (Kim and Menon, 1997), \( \sigma_{k} \) is hardwired to 1.0 like in the classical k/\( \varepsilon \) models.

In this work, a particular wall treatment was adopted, due to the necessity of capturing the effects of the swirling level imposed by the geometry. This near-wall approach is based on the work of Werner and Wengle (1991).

Boundary conditions at wall were specified by assuming that at the grid point closest to the wall, (a) the instantaneous velocity components tangential to the wall are in phase with the instantaneous wall shear stress components and (b) the instantaneous velocity distribution is assumed to follow the linear law-of-the-wall \( u^{+} = y^{+} \) for \( y^{+} \leq 11.81 \), and for \( y^{+} = y_{m} > 11.81 \) it is continued by a power-law description of the form \( u^{+} = A(y^{+})^{B} \).

The velocity components tangential to a wall at the grid point next to the wall can be related to the corresponding wall shear stress by integrating the velocity distribution over the height of the first grid element and the resulting expression can be resolved analytically for the wall shear stress component, i.e:

\[ |\tau_{w}| = \begin{cases} 
\frac{2\mu u_{p}}{\Delta y} & \text{for } u_{p} \leq \frac{\mu}{2\rho \Delta y} A^{2/3} \\
\rho \left[ \frac{1-B}{2} A^{1-B} \left( \frac{\mu}{\rho \Delta y} \right)^{1+B} + \frac{1+B}{A} \left( \frac{\mu}{\rho \Delta y} \right)^{B} \right]^{2/3} & \text{for } u_{p} \geq \frac{\mu}{2\rho \Delta y} A^{2/3}
\end{cases} \]  

(9)

Where \( u_{p} \) is the velocity parallel to the wall, \( A=8.3 \) and \( B=1/7 \) are the constants, and \( \Delta y \) is the near-wall control volume length scale.

This procedure offers the advantage that the averages \( \langle \tau_{wb} \rangle \) and \( \langle u_{p} \rangle \) are not required, and numerical problems are avoided using the relation \( \tau_{wb} = \frac{u_{p} < \tau_{wb}}{< u_{p} >} \) in reattachment regions.

In consequence of the experimental results from Ruderich and Fernholds (1986) the use of
the logarithmic-law-of-the-wall has been abandoned.

3.2 Combustion: the flamelet model
The flamelet model is one of the approaches used in the non-premixed combustion model to account for chemical non-equilibrium. The non-premixed model allows intermediate (radical) species prediction, dissociation effects, and turbulence-chemistry coupling. It is based on the assumption of equal diffusivities for all the species (generally acceptable for turbulent flows, where turbulent convection overwhelms molecular diffusion); even though in this configuration the entrance Reynolds numbers are low, the two jets impinging at 90° enhance turbulence and mixing. From the equal diffusivity hypothesis it follows that the instantaneous thermo-chemical state of the fluid is related to a conserved scalar quantity known as the mixture fraction:

\[ f = \frac{Z_{i} - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \]  

(Sivathanu and Faeth, 1990).

The corresponding Favre mean conservation equation is:

\[ \frac{\partial (\rho f)}{\partial t} + \nabla \cdot (\rho \vec{v} f) = \nabla \cdot \left( \frac{\mu_f}{\sigma_t} \nabla f \right) \]  

(10)

Defining \( f' = f - \bar{f} \), a second conservation equation for the mixture fraction variance \( \bar{f} \) can be derived and modeled:

\[ \frac{\partial (\rho f'^2)}{\partial t} + \nabla \cdot (\rho \vec{v} f'^2) = \nabla \cdot \left( \frac{\mu_f}{\sigma_t} \nabla f'^2 \right) + C_g \mu_f \left( \nabla \bar{f} \right)^2 - C_d \rho \frac{\varepsilon}{k} f'^2 \]  

(11)

The default values for the constants \( \sigma_t, C_g \) and \( C_d \) are 0.85, 2.86, and 2.0 respectively.

The mixture fraction variance is used in the closure model describing turbulence-chemistry interactions, while the flamelet concept is used to simulate chemical non-equilibrium: it regards the turbulent flame as an ensemble of thin, laminar, locally one-dimensional flamelet structures embedded within the turbulent flow field (Bray and Peters, 1994; Dixon-Lewis, 1990; Peters, 1984; Peters, 1986; Pitsch and Peters, 1998).

The chemistry can be reduced and completely described by two quantities, \( f \) and \( \chi = 2Df'f'' \) (scalar dissipation, [s⁻¹]), where \( D \) is the diffusion coefficient. This reduction of complex chemistry to 2 variables allows the flamelet calculation to be preprocessed and stored in look-up tables, thus considerably reducing the chemistry computational costs.

Since the species mass fractions and temperature in the laminar flamelets are completely parametric in \( f \) and \( \chi_{\text{st}} \), density-weighted mean species mass fractions and temperature in the turbulent flame can be determined from the PDF of \( f \) and \( \chi_{\text{st}} \) as

\[ \bar{\Phi} = \int \int \phi(f, \chi_{\text{st}}) p(f, \chi_{\text{st}}) df d\chi_{\text{st}} \]  

(12)

Where \( \Phi \) represents species mass fractions and temperature, a \( \beta \) PDF shape is assumed for \( f \) and a \( \delta \) function for \( \chi \). A simplified set of the mixture fraction space equations are solved (Pitsch and Peters, 1998; Pitsch et al, 1996).

Here, \( N \) equations are solved for the species mass fractions, \( Y_i \),

\[ \rho \frac{\partial Y_i}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial f'^2} + S_i \]  

(13)

And one equation for temperature:
\[ \rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial f^2} - \frac{1}{c_p} \sum_i H_i S_i + \frac{1}{2c_p} \rho \chi \left[ \frac{\partial c_p}{\partial f} + \sum_i \rho \chi \frac{\partial Y_i}{\partial f} \frac{\partial T}{\partial f} \right] \]  

(14)

Where \( Y_i, T, \rho, \) and \( f \) are the \( i \)-th specie mass fraction, temperature, density and mixture fraction, respectively. \( c_p \) and \( c_p^i \) are the \( i \)-th species specific heat and mixture-averaged specific heat, respectively. \( S_i \) is the \( i \)-th species reaction rate, and \( H_i \) is the specific enthalpy of the \( i \)-th species.

The reaction rate is defined by the chemical mechanism, in this case detailed, which is the GRIMech3.0 (1194).

The scalar dissipation, \( \chi \), across the flamelet, is (Kim and Williams, 1997):

\[ \chi(f) = \frac{a_s}{4 \pi} \frac{3 \left[ \rho_{\infty}/\rho + 1 \right]^2}{2 \rho_{\infty}/\rho + 1} \exp \left( -2 \text{erf}^{-1} (2f)^2 \right) \]  

where \( \rho_{\infty} \) is the density of the oxidizer stream. Note that swirl and especially curvature of micro-combustors typical geometries enhance \( \chi \) to a much larger extent than in large-scale combustors.

In this simulation 67 flamelets, with \( \chi_0=1 \) and \( \Delta\chi=2 \), have been used to describe combustion.

3.3 Numerical models

The simulation has been carried out with a Pressure-Based solver which employs an algorithm that belongs to a general class of method called the projection method (Chorin, 1968). In this method the constraint of mass conservation (continuity) of the velocity field is achieved by solving a pressure (or pressure correction) equation. This solver uses a solution algorithm where the governing equations are solved sequentially (segregated from one another) (Fluent 6.3).

The SIMPLEC (SIMPLE-Consistent algorithm) (Vandoormaal and Riathby, 1984), with a skewness correction (particularly useful with this high curvature geometry) (Fluent 6.3), is used to resolve the pressure-velocity correcting coupled equation; the SIMPLEC uses a relationship between velocity and pressure corrections to enforce mass conservation and to obtain the pressure field.

The unsteady formulation is discretized by a central 2nd order implicit scheme. The momentum equation, the energy and mixture fraction equations are discretized by the 3rd order MUSCL (Monotone Upstream-Centered Schemes for Conservatives Laws) scheme (Van Leer, 1979): this scheme is conceived by blending a central differencing scheme and a 2nd order upwind scheme. The pressure equation is discretized by a 2nd order method.

4. Results

Results are presented here that correspond to 0.0255s of simulated physical time, with a numerical time step equal to \( 5 \times 10^{-6} \)s. Results for later simulated physical times will be provided at the conference.

Figs. 4-6 show, respectively, the instantaneous temperature, the mean and the RMS at 0.0255s.

For the sake of clarity all figures show the flowfields on slices at 0.01m, 0.03m and...
0.055m, the first and last being the inlet- and outlet plane respectively.

The maximum instantaneous temperature inside the chamber is 2320K, the mean maximum temperature is 1530K, and fluctuations are of the same order of the mean value and in particular in average 1/3 of it. Fig. 4 shows also that the peak temperature is reached close to the wall, hence there are big wall heat fluxes.

The maximum temperature at the exhaust section is close to 1150K.

Figures 7 and 8 show the mean velocity map and the RMS velocity map; the comparison shows that the RMS is of the same order of the mean velocity value. This means that, in spite of the low swirl number and high temperature inside the chamber, turbulence plays an important role: this, incidentally, justifies the use of the Flamelet model.

Figure 9 and 10 show the mean Z velocity on the planes “XZ” and “YZ”. These figures
provide only negative Z-velocities, consistent with the “in-out direction” through the chamber; the black zones (positive Z-velocities) indicate the recirculation bubbles inside the chamber, important for the mixing process. This flow reversal is brought about by the shape of the geometry, in particular by the outlet section being perpendicular to the cylinder axis and tangent to its external surface (see fig. 1.).

Figures 11-12 show the mean mass fraction maps for CO and CO$_2$, the most important species for heat release.

Combustion efficiency is defined by the exhaust anhydrous molar fractions ratio, $\chi_i = n_i / (n_{\text{fuel}} - n_{H_2O})$:

$$\eta = \frac{x_{CO_2}}{x_{CO_2} + x_{CO} + x_{CH_4_{\text{load}}}}$$

The simulation predicts an efficiency equal to 0.99967.

5. Conclusions

The goal of this work was the simulation of an air/methane ultramicro-combustion chamber, designed and built at the Sapienza University of Rome, with nominal thermal power of 2KW, with the ultimate goal of supplying computational tools to design miniature electrical
power generators.

LES and Flamelet approaches have been used to simulate turbulence and combustion.

A dynamic kinetic energy transport model with an enhanced wall treatment have been used to predict the subgrid variables and velocities at wall.

67 flamelets have been used to model combustion with a detailed chemistry model: GRIMech3.0.

Results are reported at 0.025s of simulated time, and mean and/or instantaneous maps, about different variables, are provided.

The maximum temperature inside the chamber is close to 2230K while the temperature at exit is almost 1150K. The highest temperatures are close to the wall, showing high heat fluxes (critical for design procedures).

In spite of the low swirl number value (S=0.47) and the high temperatures, there are wide fluctuations inside the chamber: the maximum mean temperature is 1530K and the RMS velocity map provides values of the same order of magnitude as the mean velocities.

All this indicates that turbulence plays an important role and the non-premixed approach is reliable.

Maps of the mean Z-velocity are reported on the “XZ” and “YZ” planes: these maps show the recirculation bubbles inside the chamber, fundamental for mixing.

These recirculation zones are due to the particular geometry chosen for the chamber and it is evident that a counterflow fills wide zones of the combustion chamber, enhancing mixing and consequently the combustion efficiency, η, that is equal to 0.99967. Obviously, such a high combustion efficiency is unrealistic, and due to the neglect of external wall heat losses due to conduction, convection and radiation: we plan to include such effects in a second phase of our study and to compare the final simulation results with suitable experimental data in order to validate the computational model and to obtain useful design information.

References