Numerical modeling of steady and unsteady combustion regimes of methane-air mixture in research combustion chamber with step

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Abstract. Numerical research of non-reactive and reactive flow in research combustion chamber with step are performed. Different approaches for inert and reactive flow modeling, RANS/DES/LES, are compared and validated on extensive experimental data, profiles of velocity and temperatures are among this data. Unsteady combustion phenomena, such as flash back and flame front oscillations, are investigated and their quantitative characteristics for experimental conditions are determined. Main flow features, such as mixing layer in stabilization zone and induced by cooling system thermal boundary layer in post-combustion zone are extracted and analyzed, influence of this features on flow unsteadiness are considered.

1. Introduction

A perspective aviation engine have to meet ever more stringent requirements for emission of harmful substances and noise characteristics, as well as overall fuel efficiency. The unit of the aircraft engine, whose work directly determines the levels of emission of harmful substances and indirectly affects the noise characteristics of the engine, is the combustion chamber. The technical solutions and concepts used in such a chamber require a theoretical and experimental justification. This justification is impossible without an analysis of the complex physical processes taking place in the combustion chamber, among these processes are spraying and spreading of the fuel droplets, turbulent mixing of fuel and oxidizer volumes, turbulent combustion of fuel drop-liquid mixture. Thus, numerical modeling plays an increasingly important role in the development of new concepts of combustion chambers, most often using the apparatus of continuum mechanics and, in particular, for solving the problems of estimating emissions - the Navier-Stokes equations. However, the choice and use of certain mathematical models of turbulent reacting flow in the combustion chamber on the basis of the Navier-Stokes equations is a complex problem, the correctness and accuracy of the solution can only be provided by experiment. Therefore, each of the models used have to be verified and validated using a wide range of experimental data and conditions. It's more convenient way to start analysis of unsteady flow with combustion from simple geometry, for which detailed experimental data exists and a lot numerical research were done from different research groups. One of the possible case of such geometry is research combustion chamber with step [1] with extensive experimental data for inert and reactive flow. Thus, current work used this combustion chamber as reference point and main object for investigations. Despite the simplicity of the chosen step geometry, a lot of industrial important
physical phenomena could be observed in such geometry. Geometry is schematically depicted at Figure 1. Gaseous fuel (methane) injected through set of pylons in upstream to honeycomb (zone 1) region, mixed up with bulk airflow and then mixture are ignited by spark in after-step recirculation zone (zone 3). To avoid disturbances propagation from downstream region shutter is used (zone 2).

**Figure 1.** Scheme of ONERA A3C combustion chamber [1] configuration, numbers: 1 - honeycomb section, 2 - shutter section, 3 - step zone

2. **Numerical models and tools**

Main software tools, which were used in current work, are Computational Fluid Dynamics (CFD) codes: proprietary (ANSYS Fluent) and open-source (OpenFOAM). Reactive solvers based on control volume with unstructured and structured grids were typically selected and adapted for simulation. In addition to that, specialized software for thermodynamic and chemical kinetics calculation packages, both open-source (Cantera) and in-house are chosen for auxiliary to CFD chemical kinetics calculations. Development of mathematical models activity is focused on turbulent combustion models extension and validation for selected cases. Previously developed computationally cheap one-equation combustion model [2-5] were used for simulations and comparisons, it's based on solution of transport equation for progressive variable C. Laminar flame front velocity is pre-tabulated through 1D calculations with GRI-Mech 3.0 [6]. For high performance computations medium size distributed memory systems (up to 100 nodes) were used. Additional details about numerical procedures and hardware/software details and proposed combustion model can be found in references.

3. **Results and discussion**

3.1. **Numerical Simulation of non-reactive case**

At present, the most preferable group of methods for numerical simulation of premixed combustion is hybrid Reynolds Averaged Navier-Stokes (RANS)/Large Eddy Simulation (LES), which uses unsteady RANS near the walls (Detached Eddy Simulation, DES family) or wall-adapting local eddy (WALE) viscosity models and LES in the other regions. First series of simulations for step geometry [2], is highlighted the key role of turbulent kinetic energy budget in upstream to step boundary layer. Turbulent characteristics in combustion region after the step can't be captured with sufficient accuracy without correct description of boundary layer separation and transition zone. Since typically DES-like methods without special treatment in boundary layer, underestimate turbulent budget in RANS region, simulation with DES gives almost stationary flow near the step. To alleviate this without dramatic growth of required computational resources (Direct Numerical Simulation required about 10^{13} cells for considered conditions), wall-adapting models could be used. Boundary and mixing layer structure, underestimation and deficiency of DES-like method can be more clearly observed in non-reactive case. Simulation results in term of vorticity field and mean velocity profiles along combustion chamber for non-reactive case are presented at Figure 1. Both pictures are corresponded to mass flow rate G=0.194 kg/s, P=105 Pa, T=532 K, air-fuel equivalence ratio \( \alpha = 1.18 - 1.22 \), typical values of velocity magnitude after the step are about 55 m/s, Reynolds number based on step height equal to 4.6*10^{5}, boundary layer thickness before the step equal to 13 mm, velocity profile in boundary layer corresponds to fully developed turbulent profile. Transition from boundary layer to mixing layer can be observed at left picture, length of initially undisturbed region after the step is overestimated even for medium and fine meshes with up to 100 mln cells. But this deficiency has small impact on mean velocity profiles in after-step region. It's can be clearly seen from velocity profiles for different
sections along the combustion chamber, which are depicted at Figure 2 right picture. The discrepancies between experimental points and numerical ones is relatively small, thus overall good agreement could be observed. It's not the case for velocity fluctuations in after-step region, for which agreement isn't so good [2].

![Image](image-url)

**Figure 2.** Vorticity field in transition between boundary and mixing layers zone, ~50 mln cells, and distribution of longitudinal mean velocity, experimental and numerical, for non-reacting case at different distances X from the step, ~16 mln cells

### 3.2. Numerical Simulation of Reactive Flow with Combustion

Non-reacting case results give good starting point to simulate reactive flow with combustion. In this subsection simulations with methane combustion are considered. Simulations conditions are the same as in previous subsection, but with mixture ignition and combustion. Additional comments and remarks on computational grid size and resolution, as well as inlet boundary condition and initial turbulence intensity level discussion could be found in [4]. Typically all results in current subsection are obtained for meshes with 15.7 mln cubic cells with timestep $\Delta t=10^{-3}$ s (Courant number below unity for all cells) for unsteady simulations. It should be noted also, importance of wall cooling system modeling in sections with flame front wall attachment. Cooling of the combustion chamber walls with water was simulated using a convective heat exchange model with a heat carrier temperature of 300 K and a heat transfer coefficient on the heat carrier side of 8 kW/m$^2$K. Thermal resistance of the walls was not taken into account.

Comparison of different approaches for mean temperature profiles along combustion region is represented at Figure 3. For considered series of simulations original combustion model was used [2-5]. In addition to RANS-LES comparisons, different RANS turbulence models including Reynolds stresses model were used for testing, and they gives unsurprisingly different results [4], but the overall smallest discrepancies for temperature profiles for considered conditions gives Menter’s k-ω SST model. RANS results for mean velocity fields show good agreement with experimental profiles [4], but it's not the case for mean temperature profiles - quantitatively discrepancies could be observed in all combustion chamber zones, besides combustion zone middle section, where RANS gives good agreement as for temperature gradient, either for flame front position. As can be seen from Figure 3 in initial combustion zone computed flame front speed is sufficiently higher than experimentally measured. At the same time, at the end sections of combustion chamber, flame front wall attachment point has slightly different abscissa than experimental one. It should be noted also, that current results for 15.7 mln cells mesh show overall better agreement with experimental profiles than presented for RANS method results in [1]. Calculations using the LES WALE method on a typical grid compared to calculations on a coarse grid (3.7 mln cells) and using the RANS method give an improvement in the description of the average temperature field in the initial part and at the end of the combustion zone. However, the description of the middle part of the combustion zone has significant drawbacks - the transverse temperature gradient in the calculations is smaller, the width of the flame front is larger and its middle is closer to the bottom wall than in the experiment. In this case, the fields of averaged and
fluctuations velocities in the combustion zone correspond better to the experiment than temperature fields.

Figure 3. Comparison of mean temperature profiles along combustion zone after the step for different methods and different implementations

3.3. Numerical simulation of flashback
Numerous studies, see, for example, [7-9], are devoted to the numerical simulation of unsteady combustion regimes, including flashback, which include various methods for calculating turbulent flow and a set of models for turbulent combustion and kinetic schemes for various fuels. Application of Direct Numerical Simulation (DNS) are severely limited, since it is applicable mainly to solving model problems at small Reynolds numbers. In addition, to resolve the flame front, a grid with a cell smaller than the Kolmogorov scale is necessary, which makes this method extremely expensive. Due to the inherent three-dimensionality and non-stationarity, the LES approach provides the best starting point for modeling unstable burning modes, including flashback (flame propagation upstream to the pre-mixing section of the combustion chamber). Studies carried out over many years allowed classify the known modes of flashback in gas turbine combustion chamber [10, 11] associated with the following mechanisms: core flow flashback, combustion instability induced flashback, boundary layer flashback, combustion induced vortex breakdown. Typically in non-swirling premixed flames first three mechanisms could be observed. Due to computational efforts, required to obtain statistically quasi-stationary solution with LES, and preliminary errors estimations, associated with mesh resolution [4], small mesh with 3.7 mln cells was used in current subsection to investigate unsteady combustion regimes in step geometry.

Experimental regimes of strong oscillations of the flame front obtained in a combustion chamber with a similar geometry and parameters [12] are characterized by frequencies of 20–200 Hz. Based on computed with LES turbulence kinetic energy spectrum and compare it with theoretical law «-5/3», it can be concluded, that LES simulations well resolves the indicated frequencies of the instability modes [5]. The modes of the flame front oscillations obtained in the LES calculation is close to that observed in experiments [12] and is associated with the process of nucleation, growth and dissipation of vortices in the zone behind the step simultaneously with the pressure fluctuation. One cycle of flow evolution is represented at Figure 4, first column show relative to starting point moment in time, second column shows corresponding vorticity field, third one shows corresponding phase from [12]. At the moment the flow stagnates in the mixing channel, the flame moves forward into the channel, phase 1 in Fig.4, with the flame moving upstream into the mixing channel along the boundary layer. However, this mode does not correspond to the canonical boundary layer flashback, since the entire flow in the channel stagnates and changes direction, and in the boundary layer it occurs a little earlier. The farthest to the left position of the flame front corresponds to the highest pressure value. Then the
flame is carried downstream, pressed against the bottom wall and combustion is maintained due to the recirculation zone behind the step. For this phase of the flow evolution maximum velocity values at the end of the mixing channel and the lowest pressure could be observed, phase 3 at Figure 4.

Just as in experiments [12], it is possible to distinguish moments of time when the flame stretched by two vortices turn across the channel, phases 2 at Figure 4. It can also highlighted the moment of maximum shift of the flame front into the mixing channel when the flame front approaches the top combustion chamber wall parallel to it, and phase 5 at Figure 4. In the course of numerical simulation, effect of accelerating the flame front due to the arrival of fluid volumes with an high levels of turbulence from the mixing channel was obtained. From the data of Figure 4 it follows that at the flame front and directly in front of it at the time of phase 2 and 4 the highest level of vorticity is realized, and immediately after these phases the flame front moves as far as possible into the mixing channel. During the oscillations of the entire flow in the mixing channel at the moment of maximum velocity at the entrance to the channel, small vortices are generated. Then these vortices, developing, are transported downstream by the flow and reach the front at the time of flow stagnation. Further, the vortices dissipate, phases 2 and 5-6 at Figure 4. It should be noted that the described process proceeds simultaneously with the nucleation, growth, and releasing of vortices in the step zone. Thus, the mode with a flame front injection into the mixing channel is realized at a frequency of $\sim 32$ Hz, which is apparently related to the transfer of vortices from the computational domain inlet section to the flame front.

**Figure 4.** Flame front evolution for mixed inlet boundary condition of type $P_0^n = f(G_0)$, columns, first - point pressure oscillogram, second - field of vorticity magnitude, third - corresponding phase from [12], cinematographic schlieren photo, equivalence ratio 0.8 [12]
4. Conclusions
It was shown, that unsteady calculations of combustion processes with DES/LES approach in homogeneous combustor (step configuration, ONERA [1]) with earlier developed combustion model could describe unsteady flame front characteristics with satisfactory accuracy. Additional care need to be paid to conjugate heat transfer in hot near-wall zones and upstream turbulent intensity after the honeycomb mesh. It was shown that inlet boundary condition has significant influence on combustion stability. Unsteady regimes with flashback at frequency ~32 Hz, well corresponding with experimental frequencies, are highlighted.

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