Numerical Simulations of Flame of Single Co-Axial Injector

Victor P. Zhukov and Markus Feil
Institute of Space Propulsion, German Aerospace Center (DLR)
Langer Grund, 74239 Hardthausen, Germany

Abstract

The processes of mixing and combustion in the jet of a shear coaxial injector are investigated. Two test cases are simulated numerically. The first test case is experiments on the mixing in a non-reacting coaxial jet carried out with the use of planar laser induced fluorescence (PLIF). The second test case is experiments on the visualisation of hydrogen/oxygen flame using PLIF of OH in a single injector combustion chamber at pressures of 10–53 bar. In the first test case the simulations are performed using the shear stress turbulence (SST) model. Due to flow unsteadiness in the second test case the turbulence is modelled using transient SAS (Scale-Adaptive Simulation) model. The combustion is modelled using the Burning Velocity Model. The numerical model agrees with the experimental data very well in the first test case and adequately in the second test case.

1. Introduction

Coaxial injector has a wide usage in rocketry. It is used practically in all hydrogen and kerosene rocket engines. Though operated engines use multi-injector systems which consists of hundreds of coaxial injectors, the flame even of a single injector is an actual problem.

Tucker et al. [1] started cooperation between several institutes to compare available results of numerical simulations on a standard case, contrasting several methods with each other and with experimental data. The test case was a research combustion chamber at the Pennsylvania State University (PSU). The heat flux and wall temperature measurements by Marshall et al. [2] were used as the benchmark experimental data. In the experiment, a gaseous-gaseous coaxial injector with the similar dimensions as the SSME (Space Shuttle Main Engine) injector was tested inside the axisymmetric combustion chamber. The cooperation project consisted of a Reynolds Averaged Navier-Stokes (RANS) simulation, an Unsteady Reynolds Averaged Navier-Stokes (URANS) simulation and three different Large Eddy Simulations (LES). Different meshes with sizes between 0.25 and 255 million cells were used. The chemical reaction of propellants was modelled with the use of detailed chemical kinetics. The RANS simulation is the simplest among the performed simulations. However, RANS is not yet outdated technique and is used successfully by many researchers for simulations of flow in rocket combustion chambers. There is a big uncertainty about error sources, like mixing, heat transfer and combustion characteristics in experiment [2] that does not allow qualifying a method as incorrect in the case of disagreement with experimental data. It was shown that the results of the various codes are different with an underprediction of mixing by the RANS simulation and an overproduction of mixing with LES calculations. In terms of the heat flux at the combustion chamber walls the two-dimensional axisymmetric RANS shows the higher fluxes than the experiment, while the LES calculations show the lower wall heat fluxes. The three-dimensional simulations showed a smoother heat flux curve than two-dimensional simulations. The two-dimensional axisymmetric nature of RANS simulations implies difficulties in the mixing of hydrogen and oxygen at the centreline, hence resulting in a thin flame sheet, while unsteady simulations show a much more realistic representation of the flow.

Oefelein [3] carried out the simulations of the mixing and combustion in oxygen-hydrogen coaxial jet flames. The simulations were performed using both the large-eddy-simulation (LES) and direct-numerical-simulation (DNS) techniques employing detailed treatments of thermodynamic, transport and chemical kinetics. The modelled combustion chamber had a single coaxial injector. Cryogenic hydrogen and oxygen were injected at a supercritical pressure. The study is focused exclusively on the near-field region just downstream of the injector. The detailed numerical analysis of the flow in the wake of the injector post gave an idea about the flame holding mechanism which is provided by the strong counter-recirculating zone of hot fuel-rich products in the vicinity of the injector tip. The flame development within the stagnation region is dominated by diffusion and enhanced by convective energy transport from the backflow of fuel-rich combustion products. The backflow of hot products both sustains the flame and promotes the jet breakup of the cold oxygen core.

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Many research groups are focused on simulations of flames with liquid oxygen (H_2/LOx or CH_4/LOx flames. These works are off the scope of the current work and are not considered here. Of course, the case of combustion of cryogenic propellants is more relevant to application as the gas-gas case, but it is more complicated in modelling and in experiment. The case of gas-gas combustion has already complicated physics, so it is sensible to begin the development of the numerical model of the flow in a rocket combustion chamber from this test case rather than from the more complicated LOx case. There is also another problem associated with the LOx case. Experiments with cryogenic propellants are more difficult and more expensive, as consequence diagnostics suffer in such experiments. For example, most of the researchers, who work on modelling of cryogenic rocket combustion chambers, use "Mascotte" test case [4] for the validation. However, the experiment has provided the information only about the middle field of the flame. Such parameter as a flame length, by which a numerical model can be assessed easily, is not available in the "Mascotte" test case. By this means, "Mascotte" test case [4] is practically not suitable for the validation of a numerical model, it gives no detailed information about the flame front and gives no information about the vortex shedding and the development of Kelvin-Helmholtz instability in the wake of the injector post, that is important for turbulence and turbulent combustion modelling. Results of CFD simulations of a middle field depends more on the inlet boundary conditions, which are results of an experiment, rather than on turbulence and combustion models.
In the current work we use experiments [5,6] for the validation of our numerical model. The experimental data used here were obtained with the use of planar laser induced fluorescence (PLIF). Experiments [5,6] give more information about processes in coaxial jets than "Mascotte" test case[4], however they were carried out at injection temperature of 300 K that is limiting the validity range of tested model.

2. Modelling of mixing in the flow of a coaxial injector

To react chemically propellants should mix with each other at molecular level. In rocket combustion chamber at high pressures and temperatures chemical reactions are faster than mixing. Therefore, the mixing being the limiting stage determines the rate of the combustion process. That is why it is important to accurately model the mixing processes.

2.1 Experiments

The mixing of two gases injected by a shear-coaxial injector was examined by Schumaker [5] at room temperature in a combustion chamber at the University of Michigan. The attention was turned to the length of the inner core in dependency of the velocity and density ratios. The experimental setup consisted of a rectangular shaped "combustion" chamber (50.8 mm x 50.8 mm x 266.7 mm) with a single shear-coaxial injector. The measurements were taken at ambient conditions.
Helium and air (seeded with acetone) were used as fluids. The seeded acetone enabled the quantitative measurements of the mass fractions using PLIF in the inner jet. The experimental uncertainty amounted up to 8.2% due to the complex measurements of the molar fraction of the inner jet fluid based on the acetone. To get the quantitative data a second window was placed before the entry into the chamber to have a reference signal for the inner jet acetone concentration.
The main objective of these measurements is to obtain the core length of the inner jet, described by the position where the air acetone mixture mass fraction equals 0.89. The value of 0.89 was chosen to be equivalent to the stoichiometric line of the more interesting case of H_2/O_2 mixing. The distribution of the mixture fraction along the axis of the chamber, and also the mixture fraction distribution along the radial direction, is used to validate the numerical calculations concerning the mixing behaviour. For current work the most important test case is case C4 with a momentum flux ratio J,

$$J = (\rho_{fuel} V^2_{fuel})/(\rho_{oxid} V^2_{oxid}) = 0.42, \quad \textbf{(1)}$$

and velocity ratio K,

$$K = V_{fuel}/V_{oxid} = 0.52, \quad \textbf{(2)}$$

which are closest case to the following combustion modelling test case (J = 0.4, K = 0.4). The second in importance is case C3 with J = 1.2, K = 0.3. The overview of the conditions of the experiments is given in Tables 1 and 2.

Table 1: Injection conditions for the mixing test case.

Parameter \ Case	C1	C2	C3	C4	C5	C6
Velocity V_{fuel}, m/s	64.5	59.3	54.7	47.6	42.2	38.2
Velocity V_{oxid}, m/s	6.25	11.4	17.1	24.8	31.0	35.8
Helium mass flux φ_{fuel}, g/s	0.061	0.251	0.232	0.202	0.302	0.347
Air mass flux φ_{oxid}, g/s	0.273	0.110	0.167	0.242	0.179	0.162

Table 2: Experimental Boundary Conditions.

Parameter \ Case	Mixing test case	Combustion test case
Oxidizer injector d_i	3 mm	1.2 mm
Injector tip l	0.89 mm	0.5 mm
Fuel injector d_e	7.52 mm	2.2 mm
Temperature	300 K	300 K
Pressure	0.961 bar	10–53 bar
Momentum flux ratio J	0.13–12.3	0.4

2.2 Simulations

The simulations were performed using commercial computational fluid dynamic code ANSYS CFX [7], which utilizes the finite volume element method (FVEM). The numerical simulations of the flow inside the chamber were carried out in a 2D axisymmetric computational domain. The domain includes the injectors, but not the injector dome. In the numerical domain the turbulent flow of compressible fluid has been simulated.

The simulations were performed on hexahedral structured meshes with prismatic layers near the walls. The numerical meshes were generated using the computer program ICEM from package ANSYS CFD [7]. Six meshes with the different spacing were tested until the final mesh, which gives the mesh independent solution and has the reasonable amount of nodes, has been found. During the mesh convergence study the spacing was varied from 2 nodes at the injector post to 58 nodes. The final mesh consists of 112 thousands nodes with 29 nodes at the injector tip (l = 0.89 mm, see Table 2). The mesh is refined near the injector post and the injector walls. The expansion ratio was set to 1.2.

The flow in the combustion chamber has been modelled as a stationary solution of Reynolds Averaged Navier-Stokes (RANS) equations. The turbulence was modelled with the help of the Shear-Stress-Transport (SST) model [7] using the standard values of the coefficients and the “automatic” wall function. The transport has been modelled with the turbulent Schmidt number of 0.7 (The value of 0.7 is recommended for high-Reynolds-number jet flows by Yimer et al. [8]).

2.3 Results and Discussion

The simulations of the mixing have been used for the verification and validation of the numerical model. The flow inside the chamber is rather simple, and even the coarsest mesh gives acceptable results. Usually the details of experiments are not sufficient to establish clearly the boundary conditions (particularly the level of turbulence at inlets and thermal conditions at walls). The comparison with the experimental data helped to set the adequate boundary conditions; to choose the proper mesh; and to define the right parameters of the numerical model. Indeed the flow around the injector tip is very sensitive to boundary conditions, to numerical model and mesh.

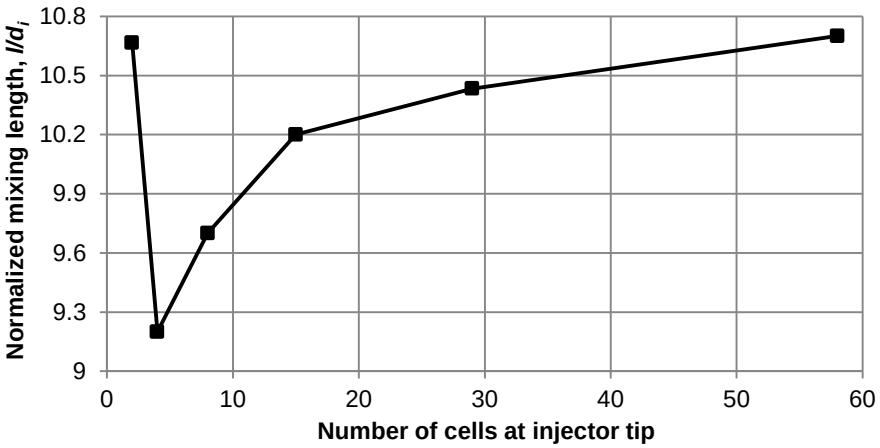

Figure 1: Mixing length as the function of mesh density, case C4.

In the work it was found (see Fig. 1) that the simulated mixing length (the distance, at which the oxidizer mixture ratio reaches 0.89) is not very sensitive to mesh density. However, as we can see in Fig. 2, the simulated flow in the wake of the injector post depends on the mesh density. The acceptable results can be obtained only on a mesh with 9 nodes at least at injector tip (In this particular case the number of nodes equals to the number of cells plus 1).

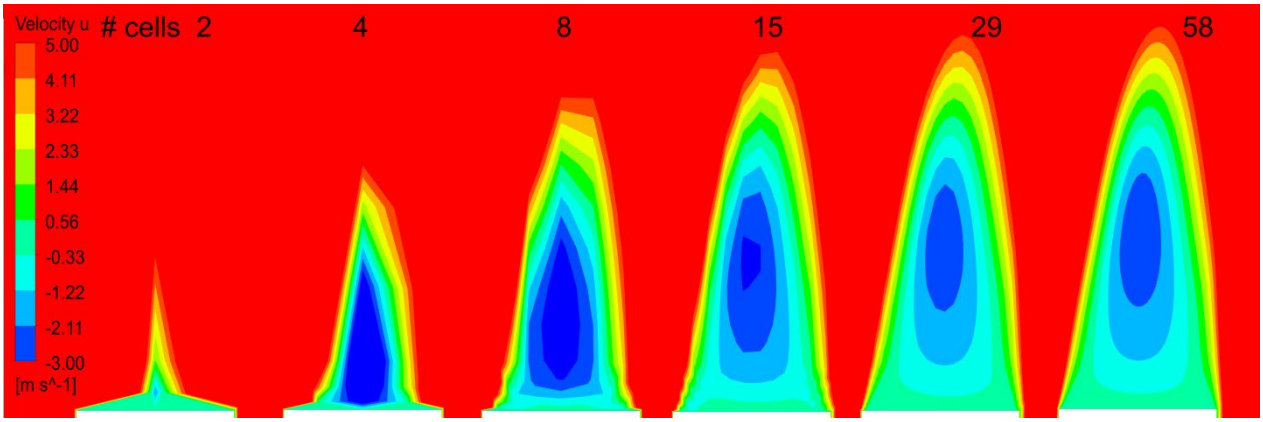

Figure 2: The change of the velocity field near the injector tip with the increase of the mesh density from 2 cells at the injector tip to 58 cells. (The red colour corresponds to axial velocities above 5 m/s, the blue colour corresponds to axial velocities below -3 m/s, the boundary conditions relates to case C4).

To obtain the good agreement with experimental data (see Fig. 3) the laminar-transition model, which is built in CFX and called “Gamma Theta Model”, has been used. The two transport equations have been employed, one for the intermittency and one for the transition onset criteria. In coaxial injectors fuel flows within a narrow gap, which amounts 1.37 mm in our case, see Table 2. In such conditions the laminarization of the flow occurs due to the viscous losses at the walls.

As we can see in Fig. 3, the numerical results agree well with the experimental data. In the both axial and radial directions the numerical model gives the distribution of oxygen which is very close to the observed distribution in the experiments (It is necessary to note that the experimental results and the simulations have the slightly different colour maps in Fig. 3). The comparison of the experiments with the simulations for all the six cases is shown in Fig. 4. For some cases the mixing is slightly overpredicted, for another it is slightly underpredicted. The experimental uncertainty amounts 8 %, so the numerical model agrees with the experiment within the measurement accuracy under such conditions in some cases, for instance in case C3 (see Fig. 5).

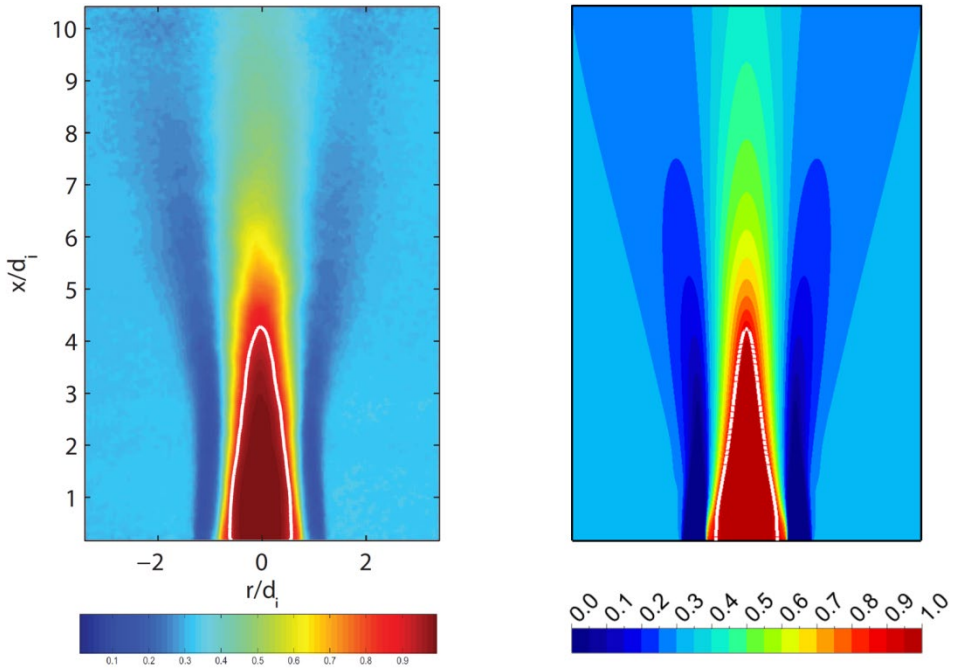

Figure 3: Mass fraction distribution for case C2, left picture – experimental data [5], right picture – simulations (The white line corresponds to the mixture fraction of 0.89).

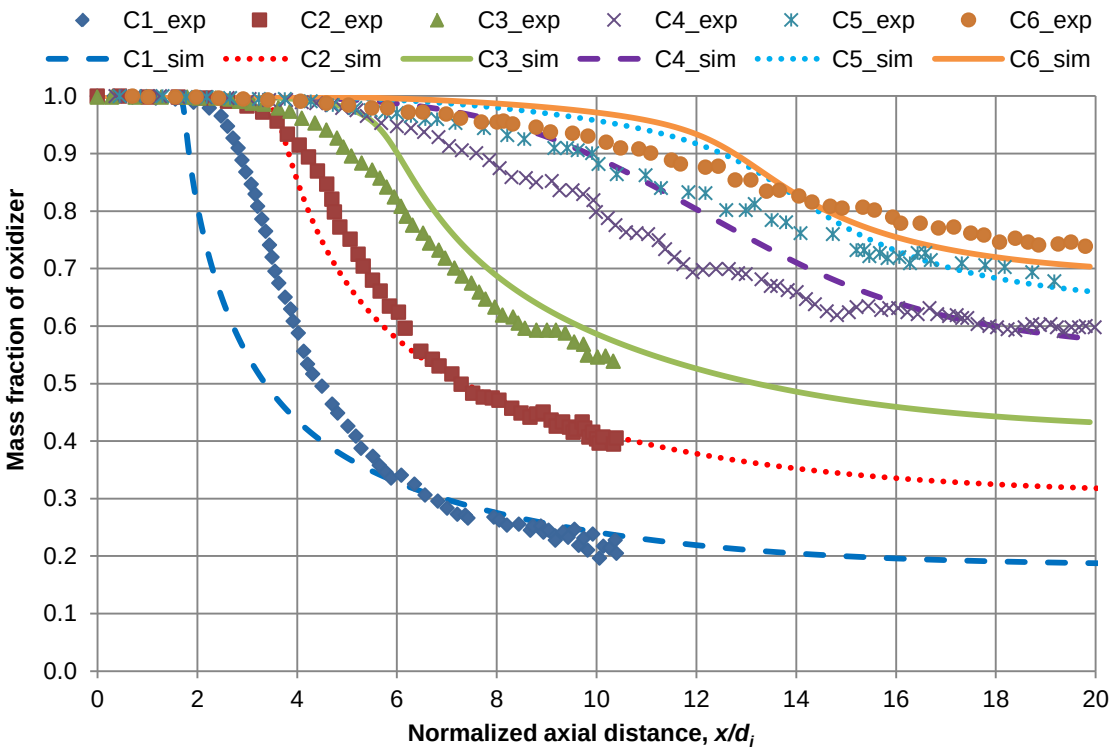

Figure 4: Mass fraction of the oxidizer at the axis of the injector as the function of the normalized axial distance (x/d_i) (symbols – experimental data [5], lines – simulations).

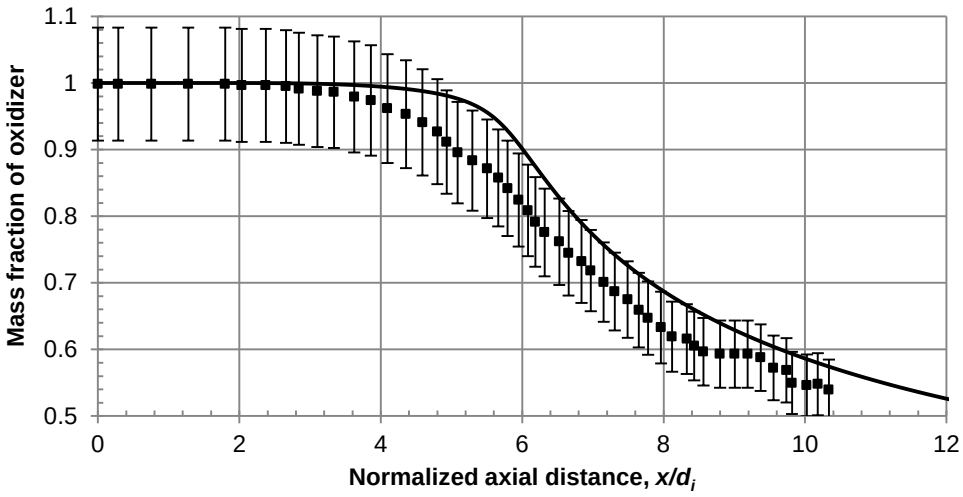

Figure 5: Mass fraction of the oxidizer at the axis of the injector (symbols – experimental data [5], lines – simulations, case C3).

The flow in the wake of the injector tip is of particular interest, because here occurs a flame holding. In Fig. 6 we see the recirculation of gas over the injector post. This recirculation is responsible for the flame holding. It provides the mixing of the reactants and captures hot combustion products. In outer flow the velocity is higher than the flame velocity. Hence, the flame cannot sustain without the flame holding provided by the recirculation zone, which is formed at the injector post edge which is the next to the flow with the less momentum. If the J number (the ratio of momentums) is close to unity, then two vortices are formed at the both edges of the injector post (see Fig. 6, case C4). The amount of gas involved in the recirculation reaches a maximum near the J number of unity. Nevertheless the J number of unity is not optimal for the flame holding. The optimum for the flame holding is reached near the J number of 10, when the gas mixture with the mixture fraction of 0.89 (i.e. the stoichiometric mixture of H_2 and O_2) is involved in the recirculation.

(a) C1, J = 12.3

(b) C4, J = 0.4

(c) C6, J = 0.13

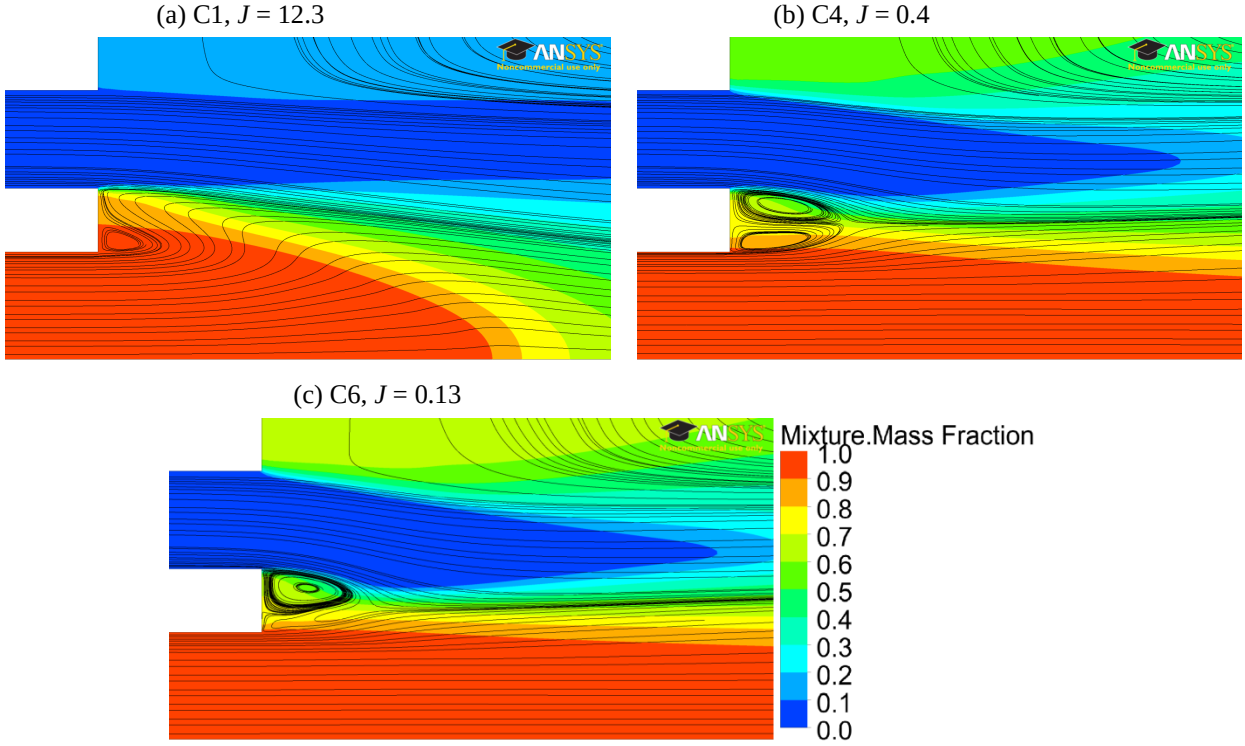

Figure 6: Flow in the wake of injector post at different momentum flux ratios. Blue colour corresponds to helium (fuel), red to air (oxidizer).

3. Simulations of the flame of a single coaxial injector

The ultimate goal of the current work is a numerical model which is able to simulate reactive flows in a rocket combustion chamber. In this case the CFD model should be validated not only against the experiments with inert gases, but also against combustion experiments. The flame of a shear-coaxial injector is a sufficiently complex object and incorporates all features of flame, so to simulate the flame of a shear-coaxial injector it is necessary to model the all properties of flame. Thus the model can be validated comprehensively the experiments on the flame of a single shear-coaxial injector. Unfortunately in most cases, when the numerical models became more complicated, the experiments provide less information.

3.1 Experiments

Vaidyanathan [6] carried out the observations of the near field of the flame of a shear-coaxial injector. In the experiments the distribution of OH radicals was measured using PLIF.
The combustion chamber has of a single coaxial injector. The chamber is made of copper and of a rectangular shape with a 25.4mm x 25.4mm cross section with large rounded corners and a modular length of up to 160 mm, depending on a measurement equipment and a test case. The injector is a shear-coaxial, with an inner diameter of 1.2 mm, an oxygen post diameter of 0.5mm and a hydrogen injector diameter of 0.244 mm. The fuel supply of hydrogen and oxygen is pressure fed, with the fluids at room temperature. There is an optical window next to the faceplate of the injector to enable measurements of OH concentration. The combustion chamber ends with a convergent-divergent supersonic nozzle which streams out into ambient conditions.
The experiments were performed at combustion chamber pressures between 10 bar and 53 bar. The test case at high pressure is only present in the current paper, see Table 3. The test duration was about 8 seconds due to heat release reasons, with the measurements taken in the last 1–2 seconds. The OH images were shot with a frequency of 10 Hz, hence nothing can be said about the temporal development of the flame. The acquired pictures can only be regarded as a random set of the instantaneous images of the OH distribution.
For the future comparison with the results of numerical simulations it is worth pointing out that the measurement error of the experimental conditions amounts 23%.

Table 3: Experimental conditions for the “combustion” test case [6].

Pressure, bar	**O/F vel. ratio**	**H_2 vel., m/s**	**O/F mass ratio**	**H_2 mass flux, g/s**	**Uncertainty, %**
53	0.40	93.4	3.85	0.75	23

3.2 Simulations

The numerical model, which had been developed for the modelling of mixing, was extended to simulate of the flame of the coaxial injector. In experiments [6] a broken flame front was observed. The broken flame front means that the flow is unsteady. (Flame in itself is the source of instability, for this reason flow is unstable in the most cases in combustion.) The RANS equations are not suitable for the modelling of unstable flows. To model the unstable flow the Scale-Adaptive Simulation (SAS) turbulence model [9] which is an improved unsteady RANS formulation has been employed. The SST-SAS model is a two-equation turbulence model, which can be operated in RANS and LES-like mode depending on the von Karman length scale and the mesh resolution. The SAS formulation introduces the additional source term into in the transport equation for the turbulence eddy frequency ω, which is defined by the von Karman length-scale. The SAS model has a LES-like behaviour in unsteady regions of the flow field (LES–Large Eddy Simulation). In regions of stable flow the SAS models switches to the SST turbulence model. To speed up the calculations the stationary solution obtained with the help of RANS was used as the initial data in the subsequent transient simulations with the use of the SAS model.
The combustion process has been modelled using the assumption of thin flame. The mixture composition is modelled using a flamelet approach. To couple laminar flamelet with turbulence the mixture fraction is integrated over the probability density function (PDF). The flame propagation was modelled with the help of the burning velocity model (BVM), also called Turbulent Flame Closure (TFC). The BVM uses an algebraic correlation for modelling the turbulent burning velocity (propagation speed of the flame in turbulent flow). The advantage of the flamelet

approach is the possibility to evaluate the mass fraction of intermediate species such as OH or other radicals and therefore to perform the comparison with optical measurements.
The mesh convergence study had been performed before the final simulations. The study gave results similar to the previous test case.

3.3. Results and Discussion

The performed simulations gave a new angle on the experimental data. In experiments [6] OH images were acquired at the rate of 10 Hz with 100 ns exposure time. The results of OH measurements are shown in Fig. 7. The advection time in the field of vision amounts 20 ms. The chemical time scale is ≥300 ns. Therefore the "instantaneous" OH image is really instantaneous. During the experiments thirteen OH images were acquired for each hot run, but the frame frequency was too low. So the all thirteen images are the set of the absolutely random shots. Thus the "average" OH image is truly average, but with the poor statistics. The comparison of the instantaneous and average image results in a fact that the flow is something in between unstable and steady flows.

Figure 7: Instantaneous (left) and average (right) OH number density contours at pressure of 53 bar [6].

In experiments [6] it was believed that the experimental data would be used for the quantitative comparison with the results of CFD simulations. The equilibrium mass fraction of OH reaches the value of ~0.12 in hydrogen-oxygen flames at high pressure. This fraction corresponds to the OH concentration of ~$15000 \cdot 10^{15}$ molecules/cm^3 in our case. The measurements underestimate the OH concentration by orders of magnitude in the flame, see Fig. 7. The conversion of the fluorescence signal into the OH concentration is complicated and it is unlikely that the error could be found at the moment. On the other hand the window in the combustion chamber is rather short and the low concentration of OH observed in the experiments may means that the flame actually ends further downstream outside the window. In the extensive study of high pressure rocket combustion by Smith [10] the flame length exceeds 120 mm in a wide range of parameters.

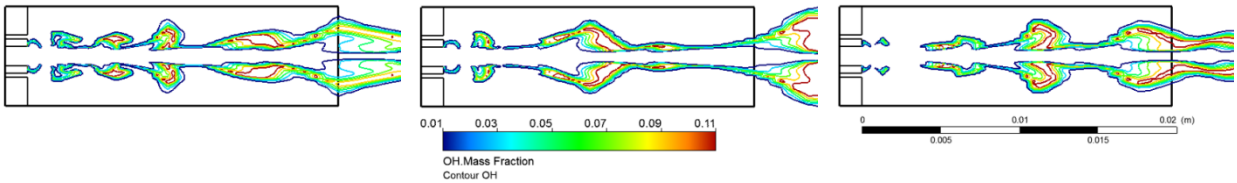

Figure 8: Instantaneous simulated OH distribution at three time moments with the interval of 0.5 ms. The black rectangle represents the borders of the window in the experiments.

The results of simulations in the 2D axisymmetric domain are shown in Fig. 8. The distinctive feature of the axisymmetric computations is the absence of the flame (OH) on the axis due to the specific boundary conditions. The flame holding occurs in the stagnate region behind the injector post. The pockets of the burnt gas arise in the wake of the injector tip, grow and travel further downstream. They pass approximately a half of the window within 0.5 ms (the time interval between shots in Fig. 8). The burnt gases separate the reactants and prevent their mixing. The reactants need a larger length for the mixing. The flame generates fluctuations in the flow which accelerate the mixing in this case. In the simulations the power of the fluctuations is less than in the experiments, because there is one degree of freedom less in the two-dimensional domain. 2D axisymmetric domain restricts the formation of turbulence structures in the circumferential directions. Under such conditions the SAS model results in a URANS-like solution (URANS – Unsteady RANS).

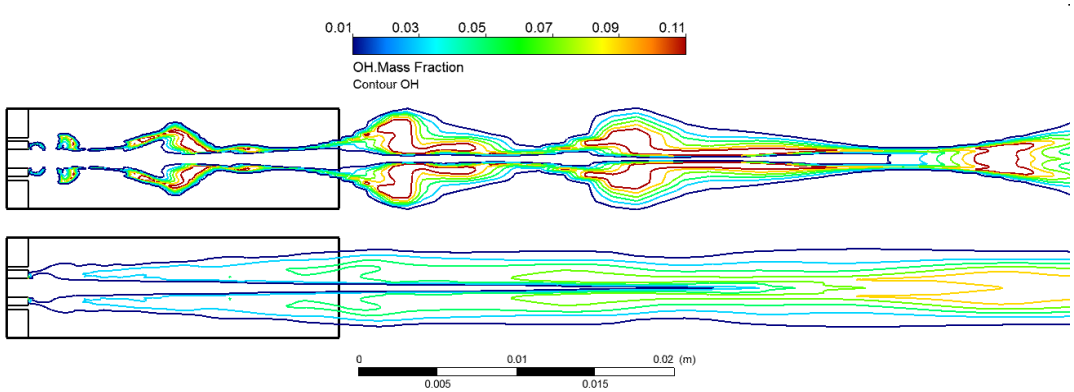

Figure 9: Instantaneous (top) and time-average (bottom) OH contours computed in 2D axisymmetric domain.

In the 2D simulations the main actions take place further downstream. The average maximum of OH fraction lies far downstream, see Fig. 9. Unfortunately the experimental data do not allow to evaluate the real flame length due to the small length of the window.

Although the quantitative comparison between the experimental results and the simulations makes no sense, the qualitative comparison is sensible. The 2D simulations visibly differ from the experimental observations unlike the 2D simulations in the previous test case. In contrast to the previous test case the fuel is separated from the oxidizer by the layer of hot water vapour now. The layer of burnt gases prevents mixing, but the higher injection velocity and the heat release in the flame result in shedding of vortices from the recirculation zone near the injector tip. These eddies make the main contribution to the mixing of the propellants.

In order to get more realistic results three-dimensional simulations have been performed. The employed 3D computational domain represents a half of chamber dissected in the longitudinal direction. The 3D numerical model does not constrain turbulence by symmetric boundary conditions thus it gives more realistic results. The results of the 3D simulation are shown in Figures 10 and 11.

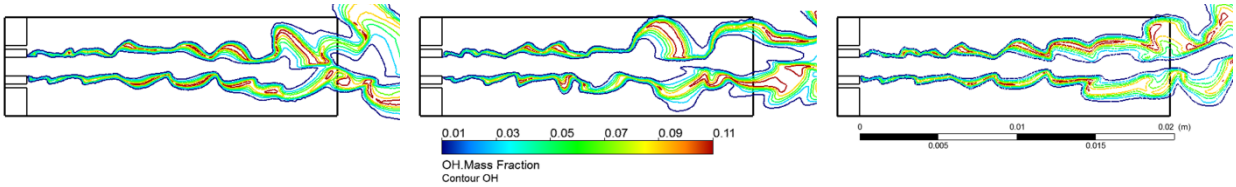

Figure 10: Instantaneous OH distribution obtained in 3D simulations at three time moments with the interval of 0.5 ms.

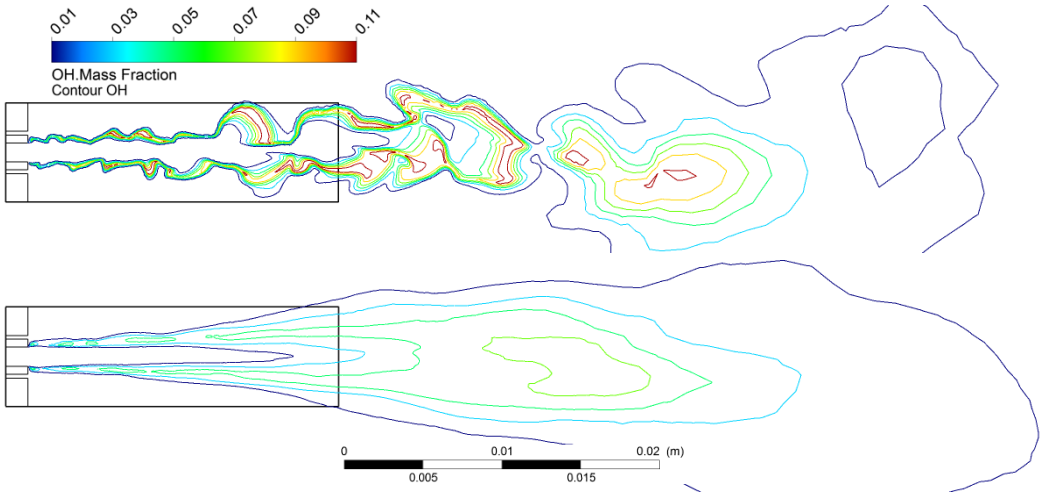

Figure 11: Instantaneous (top) and time-average (bottom) OH contours computed in 3D domain.

In the 3D simulation the frequency of the vortex shedding is higher than in the 2D simulations, vortices are smaller, but as well as in the 2D simulations the flame front is not broken in contrast to the experiments. The flame length is practically twice smaller than in the 2D simulations, see Fig. 11. In the absence of the specific boundary conditions at

the axis of the chamber the oxygen jet dissipates faster. The BVM model is not suitable for the modelling of the flames with the broken front. Therefore the further improvement requires the change of the combustion model.
The switch from the 2D computational domain to the 3D domain increased the computational time approximately in 10 times.
In spite of the similarity the test cases are characterized by the different flow fields and therefore were modelled by the different turbulence models. The velocity of "fuel" is 2 times larger in the second ("combustion") test case than in the first ("mixing") test case. Consequently, in the second test case one may expect larger in 2 times a flame length than the mixing length in the first test case. In fact the main role plays by the layer of H_2O, which separate fuel and oxidizer. This layer separates hydrogen and oxygen from each other. It even increases its thickness with the distance from the injector due to the chemical reaction. Thus the flame length ought to be very large, however there is another physical phenomenon which reduces the flame length in the second test case. The large gradients of density and velocity in the flow result in a strong Kelvin–Helmholtz instability in the second test case. In the first test case the density gradients are 100 times smaller (the velocities gradients are smaller too, but only 2 times) and the Kelvin–Helmholtz instability was not observed in experiment [5]. In the second test case we have additionally the layer of hot water vapour with the very low density. The presence of the Kelvin–Helmholtz instability leads to the necessity for the use of a scale resolved turbulence model (SAS, DES, LES, etc.) what in turn requires the use of a 3D numerical domain.

4. Conclusions

The mixing and combustion of the propellants injected by a single shear-coaxial injector have been simulated using the CFD code ANSYS CFX. The numerical results have been compared with the results of the experimental observations.
The mixing in the jet of coaxial injector has been modelled using the stationary SST turbulence model in the 2D axisymmetric numerical domain. The numerical results agree with the experimental data very well.
In the both test cases the mesh study showed that the numerical grid needs 8–15 nodes at the injector tip to form the recirculation zone over the tip and 15–30 nodes to get a mesh independent solution.
To simulate the flame the numerical model was extended by the BVM combustion model and the unsteady SAS-SST turbulence model. In contrast to the mixing test case the results of the flame simulations are not clear. The experimental results do not allow performing the direct comparison with the numerical results due to the incorrect values of OH concentration estimated in the experiments.
The flame of a coaxial injector is held in the stagnation region behind the injector tip. In the flame the propellants are separated by the layer of burnt gases. The numerical model, which agrees well with the experiment in the simulations of the flow of non-reacting gases, gives the large mixing length (large flame length). The mixing length is shortened approximately twice using the three dimensional numerical domain in the simulations. The 3D numerical model produces more realistic results than the 2D model. However, the developed 3D numerical model still is not absolute. The employed BVM model does not reproduce the broken flame front, which was observed in the experiments. For this reason the further improvement of the numerical model requires the abandonment of the thin-flame assumption.
The comparison of the studied test cases emphasizes the complexity of flame simulations. The layer of hot gases produced in chemical reaction results in the onset of the Kelvin–Helmholtz instability while CFD simulations of flow instabilities are much more complicated than simulations of stationary flows.

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