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NON-REACTIVE FREE JET FLOW: COMPARISON OF SIMULATIONS USING DIFFERENT TURBULENCE MODELS WITH REFERENCE MEASUREMENTS

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Abstract. *Hot free jet flow is an important process in risk assessment and explosion protection in various ranges of application. The numerical study on nonreactive jets with fully developed turbulence and density variations were performed using different turbulence models. As expected LES simulations give best result but are highly time-consuming. When the parameter of the SAS model will be adapted to the free jet problem SAS could be a feasible alternative with smaller expense. The lower resolution of URANS models may be sufficient for problems with moderate Reynolds number. In accordance with the measurements based on LIF technique numerical simulations characterize a pulsed helium free jet injected in nitrogen. A moderately turbulent flow is evaluated by URANS simulations conform to measurement data.*

1 INTRODUCTION

Unsteady jets with density variations are found to be a fundamental situation in applications especially in combustion systems and explosion protection equipments. In order to control the ignition of fuel/air mixtures besides the chemical interaction the knowledge of the mixing process and the mixture fractions are important prerequisites. The mixing process between emerging jets and the surrounding is of special interest concerning the autoignition inside internal combustion engines[4,9].

Numerical studies on non-reactive jets with density variations were performed using a Reynolds model[6] and in recent time using large-eddy simulations[7,13]. As advantage, the numerical simulations would provide the opportunity of detailed studies on the mixing and interaction process. On the other hand,depending on the turbulence models may be yielded different results. This problem can be solved by comparisons with reference measurements. However, a comparison of different turbulence models is pending.

Furthermore, experimental studies on turbulent round jets widely exist but relatively few on jets with variable density (e.g. see [1,2,11,12]). A helium jet impinging in air or other gas mixture is typically used in variable density jets which conforms to our experimental setup. Here, a Fuel Stratified Injection (FSI) valve is used to expand pre-compressed helium in a pre-chamber to ease the flow, after which the gas mixture enters a pipe[8]. The transient jets caused by a pulsed injection at the nozzle outlet are produced with a repetition rate of 1 Hz and high reproducibility, respectively. The mixing process between free jet and quiescent nitrogen atmosphere is examined using nitric oxide (NO) as tracer molecule for quantitative measurements.

First, the measurement arrangement is presented which were performed in the framework of explosion protection. Some basics about the relevant turbulence models and the numerical setups are given in section 3, here we use URANS (unsteady RANS), SAS (Scale-Adaptive Simulation) and LES (Large Eddy Simulation) compared with LES results from[13]. The results are presented in section 4 for the two cases with different momentum flux at the outlet of the pipe. Finally, conclusions are drawn.

2 EXPERIMENT

Helium, nitrogen and argon jets have been examined experimentally to yield information about the interaction of variable density jets with a quiescent surrounding of nitrogen[8]. The density ratio was varied from 0.14 (helium/nitrogen), 1.0 (nitrogen/nitrogen) to 1.4 (argon/nitrogen). Helium, nitrogen and argon jets have been examined experimen-

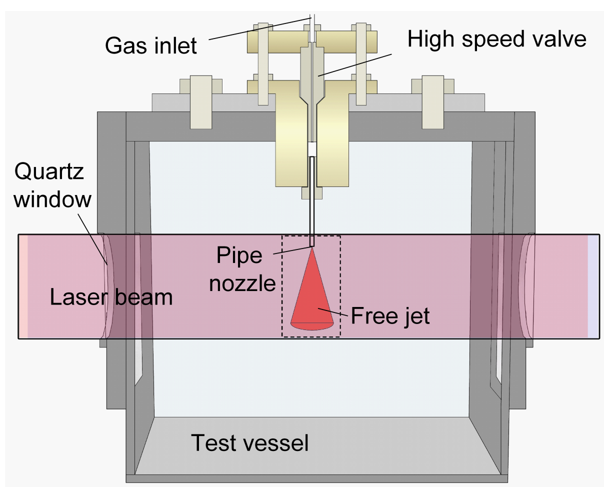

Figure 1: Experimental setup.

tally to yield information about the interaction of variable density jets with a quiescent surrounding of nitrogen. The density ratio was varied from 0.14 (helium/nitrogen), 1.0 (nitrogen/nitrogen) to 1.4 (argon/nitrogen). The experimental setup shown in figure 1 consists of a vessel with a volume of 12 l. The dimensions of the test vessel are large in relation to the jet to avoid a significant impact from the walls of the vessel. The test gases, having a reservoir pressure of up to 7 bar, are expanded using a Fuel Stratified Injection (FSI) valve. The trigger signal of the valve has a jitter of 10 µs with respect to the data acquisition. The quantity of injected gas is a linear function of the injection duration[8]. A pipe nozzle 70 mm in length with a diameter of 1 mm is used to generate subsonic free jets.

The test vessel is equipped with quartz windows, which offers the possibility to examine

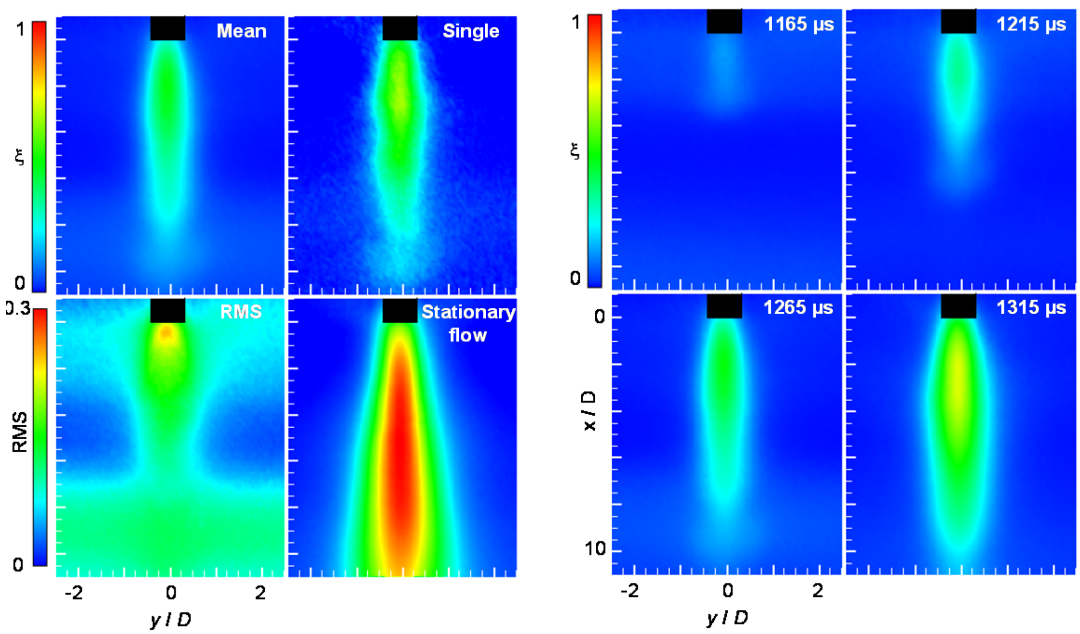

Figure 2: **Left:** 2D distribution of the molar mixture fraction ξ (Helium jet, inlet pressure 4 bar, t=1265 µs). **Right:** Temporal evolution of mean molar mixture fraction fields ξ (Helium jet, inlet pressure 4 bar).

the gas injection and mixing processes in detail. Therefore, the test vessel was filled with nitrogen including 1000 ppm oxide. The interaction between gas jet and quiescent nitrogen are examined using quantitative measurements by means of laser induced fluorescence of NO. Molar mixture fraction maps are yielded. Here, mixture fraction ξ is defined as the fractional part of gas origination from the jet. More details about the experimental setup can be found in[8].

At defined times after opening of the FSI valve 100 injections have been examined for each configuration, which offers conditional ensemble statistics[4]. Figure 2 left shows typical results for a helium jet with an inlet pressure of 4 bar at t = 1265 µs. Averaging the 100 single measurements yields a smooth mean mixture fraction field. However, each instantaneous measurement as given in figure 2 left shows turbulent fluctuations. Mixture fraction fluctuations up to 25 % can be seen from the rms values in figure 2 left. The mean mixture fraction map of the stationary flow is also shown in figure 2 left.

The phase-averaged evolution the mean molar mixture fraction using helium with an inlet pressure of 4 bar is shown in figure 2 right. From these measurements, e.g. radial distributions can be yielded, which shows Gaussian distribution with respect to time and space[8]. The experimental results can be used to derive local distributions yielding probability density functions of the molar mixture fractions based on a statistical analysis. However, numerical simulations of these variable density jets as presented in this paper are necessary to validate the experimental results.

3 NUMERICAL METHODS

In the described experiment we deal with a Newtonian fluid which is governed by the Navier-Stokes equations

$$\begin{aligned} \frac{\partial}{\partial t}\,\boldsymbol{U} + (\boldsymbol{U}\,\mathrm{grad})\,\boldsymbol{U} + (\frac{1}{\rho})\mathrm{grad}\,p &= \nu\Delta\boldsymbol{U} \\ \mathrm{div}\,\boldsymbol{U} &= 0 \end{aligned} \tag{1}$$

for the velocity $\boldsymbol{U}$ and pressure p. Because we examine a helium-nitrogen mixture one transport equation for the mass fraction of helium C_{He} has to be added

$$\frac{\partial C_{He}}{\partial t} + \boldsymbol{U}\,\mathrm{grad}\,C_{He} = D_{He}\Delta C_{He} + Q(t,\boldsymbol{x}) \tag{2}$$

with a diffusion coefficient D_{He} and source term Q which is equal to zero in our application. The geometrical model as shown in figure 1 we reduced to a pipe with a length of 7 cm and a diameter of 1 mm and the pre-chamber was omitted. The simulations were divided into two steps. First, the simulation of the nitrogen flow inside of a shorter pipe (7.5 mm) with periodic boundary conditions were performed. After four reruns a fully developed velocity profile is reached which are retained unchanged in further iterations. In this way we drastically cut down on computing time compared to a simulation with the real pipe geometry. In the second step the free jet is simulated with velocity boundary conditions at the inlet of a shorter pipe (1.5 mm) corresponding to the result of the first step. For the mass fraction of helium C_{He} at the inlet we have as unsteady boundary condition a step function. After a pure nitrogen pre-flow of $t_p = 2\,\mathrm{ms}$ the inlet flow switches to a pure helium flow.

$$\begin{aligned} C_{He}(t) &= \begin{cases} 0 & \text{if } t < t_p \\ 1 & \text{if } t \geq t_p \end{cases} \\ C_{N_2} &= 1 - C_{He}\ . \end{aligned} \tag{3}$$

The temporal evolution of the helium distribution in nitrogen after the helium injection is investigated by computer simulations in analogy to the experiment. The solution of the Navier-Stokes equation known as direct numerical simulation (DNS) resolves all length scales and timescales and represents a single realization of the flow with the disadvantage of extremely high computational effort. Because the Reynolds number at the nozzle aperture ranges moderately between 1500 and 2000 the Unsteady Reynolds averaged Navier-Stokes (URANS) with the shear stress transport model (SST)[10] are applied. This turbulence model splits the flow variables into one time averaged (mean) part and one turbulent part. Unlike the RANS model the URANS averaging is carry out over a narrow time interval.

Moreover, instead of adjusting the results by experiments a verification can be achieved by comparisons with results found in the literature. According an idea given in[2] flow regimes with identical momentum flux M

$$M = 2\pi \int_0^\infty \rho\, U^2 r \cdot dr = \frac{\pi\rho\, U^2 D^2}{4} \tag{4}$$

are well comparable for instance for velocity profiles or density distributions, both normalized to the corresponding values at the nozzle tip. D is the nozzle diameter and ρ the fluid density at the nozzle. In[13] a free jet caused by an helium injection in air with momentum flux $M = 0.1$ is detailed discussed, both LES simulations and experiments.

The geometry and computation domains of both free jet simulations are composite in table 1.

geometry	D	L	x (streamwise)	y (radial)	z (radial)	elements
G1	1.2 mm	70 mm	$58D$	$40D$	$40D$	4.9 mio.
G2	26 mm	200 mm	$40D$	$11D$	$11D$	8.4 mio.

Table 1: Computational domains with nozzle diameter D, nozzle length L. G1 - geometry of our experiments, G2 - similar geometry to the configuration in[13] but in absence of a weakly confined co-flow.

Higher Reynolds number suggests the application of more precise turbulence models. The immense expense of DNS can be avoided using the large-eddy simulation (LES)[5], where the Navier-Stokes equations are solved for a filtered velocity field which presents the motion of the large eddies and the small scales are considered by an eddy-viscosity model. The filter scale determines the resolution of the motion, but very small scales are associated with strongly increasing expense. The relatively new Scale Adaptive Simulation (SAS) adjust the turbulence length scale to the local flow inhomogeneities[3], which is based on the introduction of the von Karman length-scale into the turbulence scale equation and on the SST-model. SAS models can produce the entire range of solutions from LES to steady RANS by simply increasing the time step. The simulations were performed with the software package ANSYS CFX.

4 Results

As described above the numerical simulations are arranged in two groups both for variable density flow. First, for comparisons with results in the literature[13] we chose a configuration with the same momentum flux M from equation (4) at the jet exit according to an idea in[2]. The simulations based on geometry G1 and on geometry G2 (see table 1) and $M = 0.1$ are compared using the different turbulence models URANS, SAS and LES. In group two URANS simulation of a pulsed free jet combined with geometry G1 is discussed in comparison with measurement data.

4.1 Fully turbulent jet simulations with URANS, SAS and LES

For our comparisons the LES results from[13] were involved which had been verified by experiments. Therefore our LES simulations are indirectly compared to experiments, too. Their geometry G2 and our geometry G1 are given in table 1 and the associated stationary flow regimes in table 2. Because of the equal momentum flux equation at the nozzle (4) the regimes are comparable in some respects.

For geometry G1 the velocity at the nozzle U_0 was set to 738 m/s. This leads to a Mach number of 0.76 considering the sound velocity in helium of 970 m/s. For gas flows where the Mach number exceeds 0.3 ANSYS CFX holds a *Total Energy* model which includes the transport of enthalpy and kinetic energy effects.

flow regime	geometrie	M (N)	U_0 (m/s)	ρ_{He}/ρ_{N_2}	M_a
F1	G1	0.1	738	0.14	0.760
F2	G2	0.1	32	0.14	0.033

Table 2: Parameters of the both flow regimes. F1 corresponds our experimental geometry G1, regime F2 to[13].

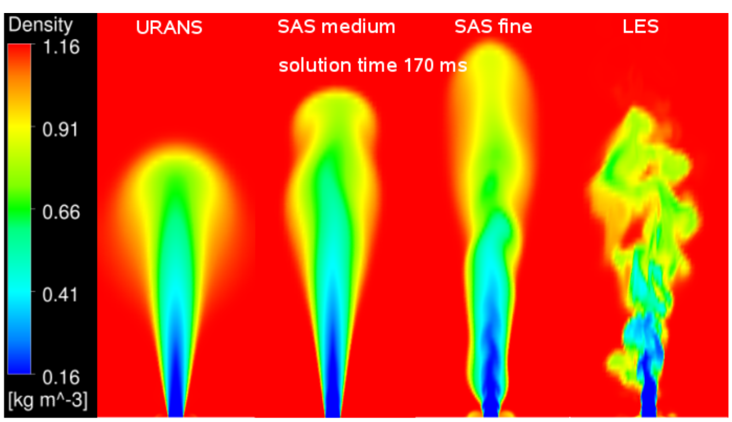

Figure 3: Simulated density in the transient regime of the transient free jet (helium jet injected in air) according regime F2 after 170 ms for different turbulence models: URANS, SAS with medium time step, SAS with fine time step, LES.

The numerical simulations were performed using a selection of different types of turbulence models: URANS, SAS and LES as described in section 3. For LES we chose the Smagorinsky subgrid-scale (SGS) model. The default value of C_s was decreased to 0.085,

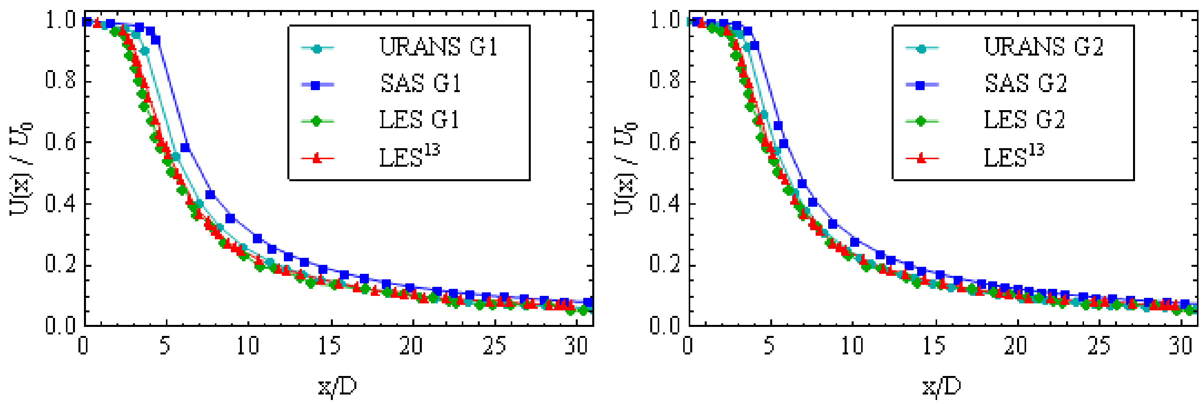

Figure 4: Mean velocity along the jet axis for different turbulence models. The special curve LES[13] was taken from[13] belonging to F2. **Left:** RANS, URANS and SAS for regime F1 (except LES[13]) . **Right:** URANS, SAS and LES for regime F2.

because it is not an universal constant and depends on type of flow and mesh resolution. Furthermore we changed the turbulent Schmidt number S_c to 0.7 as proposed in[13].

Figure 3 shows the density distribution after 170 ms for flow regime F2 simulated with different turbulence models. The scale reaches from the density of helium 0.16 kg m^{-3} to the density of air 1.6 kg m^{-3}. As expected the eddy resolution will be higher from the left simulation to the right, from URANS to LES, SAS is in between. Moreover, axial profiles of the velocity and the mass fraction provide more precise information.

In figure 4 the mean streamwise velocity profiles are given for both flow regimes F1 and F2 simulated with different turbulence models. Interesting, both families of curves are virtually identical, for example the curves LES G1 and LES[13] at the left side are hardly distinguishable. The reasons are the same momentum flux and of cause the normalization. Otherwise, the length of the core region of the helium jet is simulated different for the three models as figure 3 already suggested. LES leads to a length of 3 diameters, SAS to a length about of 5 diameters and URANS lies in between. The difference of the SAS result could be caused of the fact that the validation of the SST-SAS model with optional parameters mainly concerns aerodynamic applications. The parameter adaption to the free jet problem will be a future task.

As shown in figure 5 left the mean mass fractions have the same trend depending on the turbulence model. The normalization constant $C_{He,0}$ is the mean mass fraction of helium at the nozzle. The radial profiles of the normalized velocity displayed on right side of figure 5 are in a good agreement where the space normalization is done by the half-width of the velocity L_u .

Figure 4 and 5 show the properties on the symmetrical axis but the half-widths given in figure 6 tell about the spreading rate. When we state the results in[13] and[1] as verified than the URANS simulation overestimate the spreading rate on the other hand SAS underestimate the rate (may be cause by the overestimated core). Our LES results agree

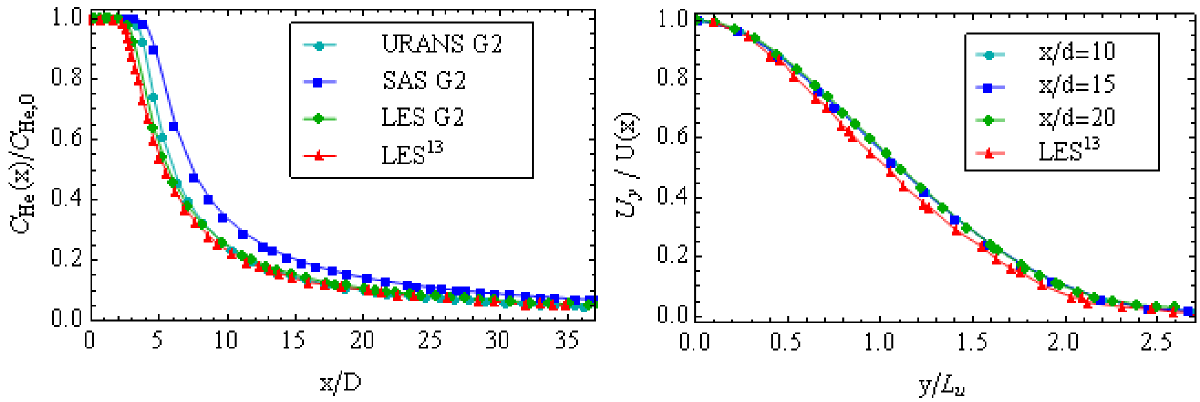

Figure 5: **Left:** Mean mass fraction of helium along the jet axis for different turbulence models. Regime F2 is used for URANS, SAS and LES. **Right**: Radial velocity profiles at various distances from the nozzle tip. URANS for regime F2 is used.

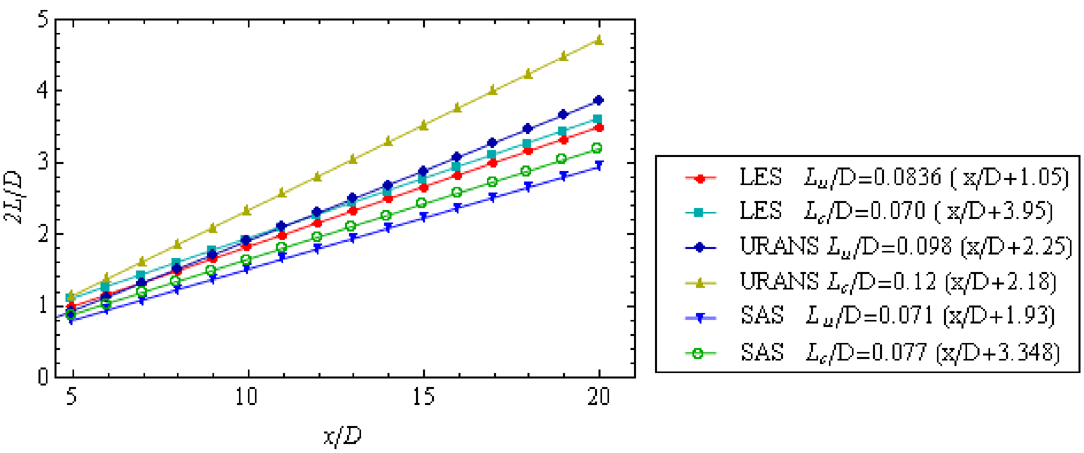

Figure 6: Half width of the mean streamwise velocity and of the mean mass fraction along the jet symmetry axis for the flow regime F2.

with[13]. L_c, the half-width of mass frction is always greater than L_u because of the shift of the virtual origin (x_u and x_c). The velocity field always spreads slower than the scalar concentration field.

4.2 Pulsed free jet: simulation - experiment

As mentioned in section 3 the fluid flow in the pipe was effectively calculated by a pipe segment with periodic boundary condition* and the pre-chamber was omitted. Because of the relatively low Reynolds number URANS was chosen to simulate transient variable density jets. Due to the complex experimental setup, no detailed information about

*The implementation in CFX is carried out using a domain interface with *translational periodicity* for periodic boundary conditions.

the inlet conditions with respect to velocity and pressure exists. Therefore, these inlet conditions have been varied until a satisfying consistency of axial and radial profiles of molar fraction at selected positions has been yielded, which gives an outflow velocity of approximately 145 ms. A comparison of molar fraction profiles for different distances from the nozzle tip was necessary for the numerical adjustment of the measurement position. The radial profiles at $x = 5$ mm, 6 mm and 7 mm show an earlier helium saturation. The best fit was reached at $x = 8$ mm, see figure 7. The observation profile in the experiment is positioned at $x = 5$ mm.

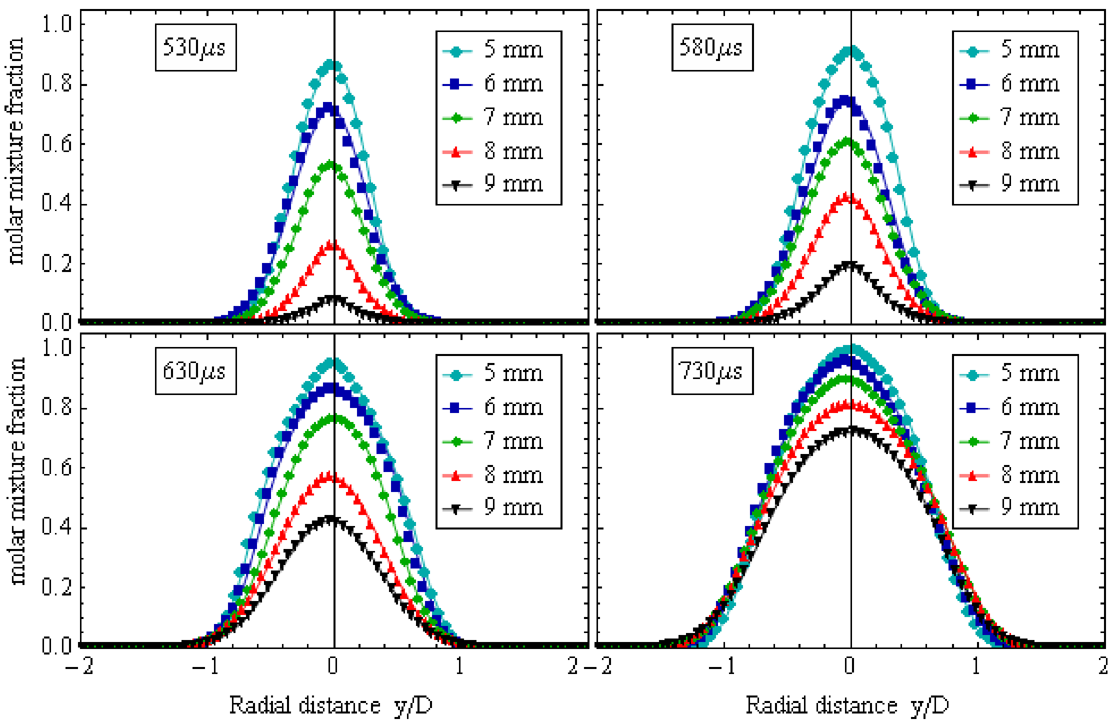

Figure 7: Comparison of simulated molar fraction profiles of helium for each time at different distances from the nozzle tip. The times are chosen to be the same as in figure 8.

Certainly, the absolute times do not coincide because the simulation did not incorporate the pre-chamber and the full length of the pipe, see figure 1. A time difference of 685 µs corresponds to the way through the equipment. It is more important that the relative times are identical. As shown in figure 8 the temporal evolution of the molar fraction field can be described sufficiently using a specific inlet condition. However, as can also be seen in figure 8, differences as the spreading rate exist between simulation and experiment which are subject of further investigations.

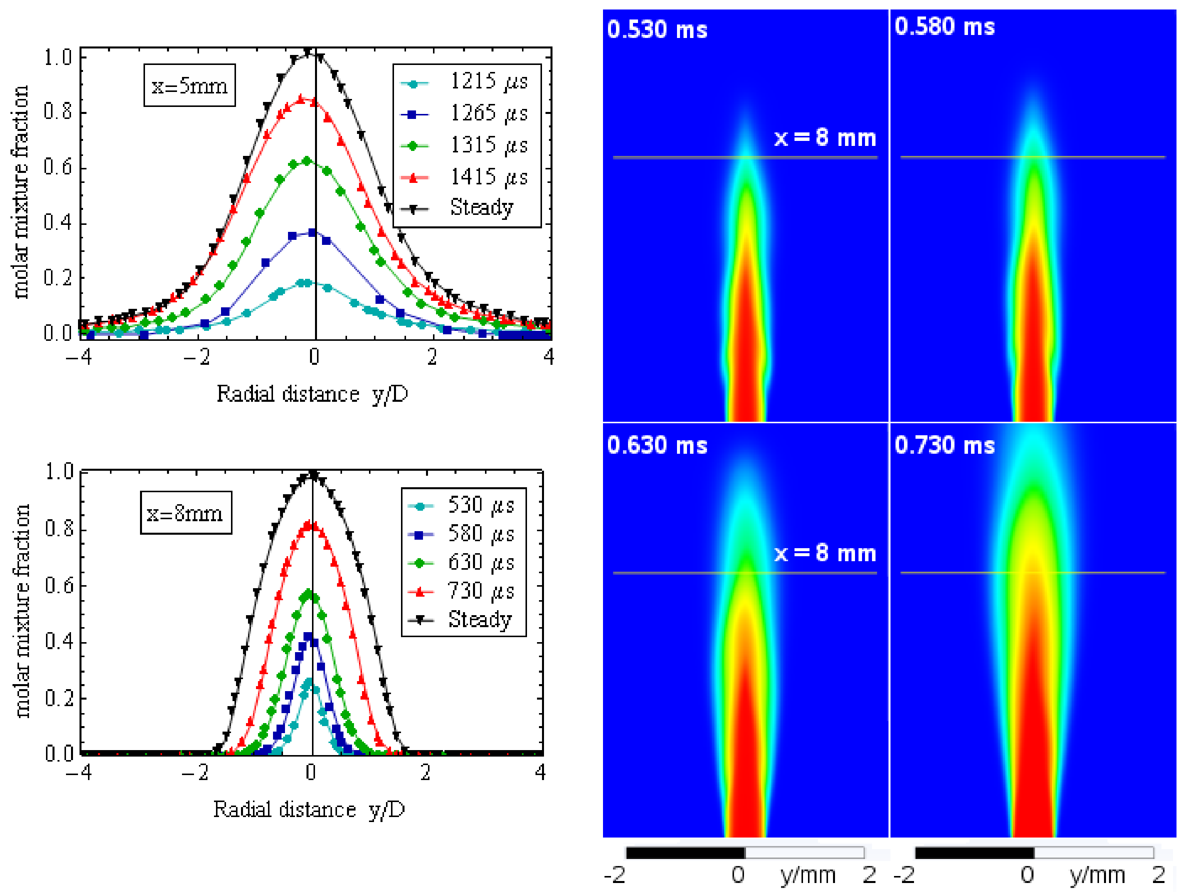

Figure 8: Temporal evolution of the mean molar fraction of helium. **Left:** Above - Measurements corresponding to figure 2 right. The observation profiles in the experiment are given at $x = 5$ mm. The time differences are 50 µs, 50 µs and 100 µs, in all 200 µs. Left: Below - URANS simulation. The temporal evolution was best fitted to the experiment at $x = 8$ mm. **Right:** Cross section of the simulated molar fraction for the same times as left.

5 CONCLUSIONS

The ignition process in transient free jets depends on a complex interaction of turbulent flow and chemical kinetics. Computer simulations yield to a good insight into the properties of the fluid flow and may contribute an important part to a risk analysis for many applications.

The numerical study on nonreactive jets with fully developed turbulence and density variations were performed using different turbulence models. As expected LES simulations give best result but are highly time-consuming. When the parameter of the SAS model will be adapted to the free jet problem SAS could be a feasible alternative with smaller expense. The lower resolution of URANS models may be sufficient for problems with moderate Reynolds number. In the experimental part of work LIF technique was used for measurements of the evolution of pulsed helium free jets injected in nitrogen which causes a rarely investigated variable density flow with moderate turbulence level. In accordance with the experiments computer simulations based on the URANS turbulence model achieved results conform to measurement data.

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