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Numerical analysis of an impact of spray characteristics and co-flow temperature on a flame lift-off height

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Abstract. In the current work the jet spray combustion reflecting an experimental piloted spray burner is simulated numerically. In the simulations the diluted ethanol spray evaporates in the hot surrounding, the gaseous fuel diffuses from spray fuel-rich core into the oxidizer fuel-lean region and autoignites. An in-house high-order compact difference LES solver is used to carry out the computations. The reaction rates are modelled using Implicit LES approach based on the single-step global reaction. The continuous phase is modelled in the Eulerian reference frame while the droplets in the Lagrangian form. The studies are focused on the influence of the co-flow temperature and spray initial Sauter mean diameter (SMD) on the flame lift-off height, autoignition delay and the reaction zone features. The results are compared with the experimental data and show good agreement in terms of lift-off height. It is almost linearly related to the co-flow temperatures. It is found that for the same fuel mass loading, droplets with smaller SMDs significantly shorten the autoignition delay. Moreover the autoignition delay and the lift-off heights are influenced mostly by the droplets SMD rather than by the co-flow temperature.

1. Introduction

The combustion processes are one of the most fundamental ways of global energy conversion. A variety of industrial and small scale devices operate being powered as a consequence of highly turbulent combustion processes that follow the liquid fuel injection, e.g., diesel engines, burners, aircraft propulsion systems, liquid fueled rockets engines and many others. The difficulties of turbulent combustion analysis in two-phase flows arise from a range of interlinked phenomena that cannot be fully captured by the experiment. These are manifested by: the turbulence, droplet dispersion, evaporation, mixing of fuel vapour and chemical reactions. Albeit the experimental and numerical techniques advancement, the two-phase combustion comprises a research field that is far from being fully understood. Numerical studies using both the Direct Navier-Stokes (DNS) [1] and Large Eddy Simulation (LES) [2] approaches enable analysis of two-phase combustion processes with precision unreachable by experiment. The DNS provides a detailed insight into flows nature but is limited mainly to flows in simplified domains and assuming low Reynolds numbers. The LES is the tool which boosts further advancements in spray combustion.



In the framework of LES, the biggest challenge in simulations of turbulent flames is proper modelling of turbulence-flame interactions at sub-grid level that influence the reaction rates. Various strategies for modelling the reaction rates can be employed, such as: Lagrangian Particles, transported PDFs, Eulerian stochastic fields along with Monte Carlo solution techniques. There are also simpler modelling methods, promising from practical point of view, i.e., implicit LES (ILES) [3]. The ILES method is particularly well suited for comparative and parametric studies of complicated reacting flows as it is robust and provides fairly reliable solutions. In the current work it is applied to study the jet spray flame surrounded by the vitiated co-flow, reflecting an experimental configuration investigated originally by the O'Loughlin and Masri [4]. The fuel (ethanol) spray is produced using the ultrasonic nebulizer and is fed to the combustion chamber. The droplets evaporate in the hot surrounding then the gaseous fuel diffuses from spray fuel-rich core into the oxidizer fuel-lean region and autoignites. We analyse the influence of an initial size of fuel droplets and the co-flow temperatures on the flame lift-off heights, autoignition delays and the reaction zone features. The results are compared with the experimental data and show good agreement in terms of lift-off height.

2. Mathematical model

Computations are carried out using an in-house academic LES solver SAILOR [5]. The code solves the LES equations [6] for low Mach number flows disregarding the acoustics modes. The derivatives in Navier-Stokes and energy equations are discretised in Cartesian coordinates using a high-order compact difference scheme [7, 8] on collocated grid arrangement and half-staggered mesh for the pressures nodes. The staggered grid arrangement ensures oscillation-free pressure field since the pressure nodes are decoupled from the values stored in the collocated grid. The pressure field is obtained from the solution of the Poisson equation. The governing equations are integrated in time with the use of predictor-corrector approach. At the predictor step, the second order Adams-Bashforth method is used and at the corrector step the second order Adams-Moulton method is applied. The dispersed phase is modelled in the Lagrangian framework where isolated droplets act on the gas phase through the momentum, mass and energy source terms. The source terms formulations in Navier-Stokes equations were drawn from [9]. Their evaluation is performed by summation over each of the droplet contribution. The equations for droplets positions, velocity and temperature are integrated in time using the 1st order Euler method. The two-way velocity and energy coupling is based on 2nd order approximation of source terms with 4th degree Lagrangian polynomial approximation of the flow field variables at the droplets positions. The numerical code was thoroughly tested and validated for various configurations including both non-reacting and reacting flows [10, 11]. For modelling the species reaction source terms we use the Implicit LES (ILES) approach [3]. The main difference between LES and ILES relies on treatment of the reaction source terms. In ILES the sub-filter scales resulting from the filtration of the convective terms are modelled by the use of eddy viscosity model, but the filtered chemical source terms are modeled directly using the large scale quantities solved on the computational mesh. In this case the reaction rates are obtained from the Arrhenius formulas and in the present study we use simple one-step chemistry for the ethanol oxidation. The reaction rates are tuned with respect to the local equivalence ratio such to reflect correctly the extinction limits.

3. Configuration

The computational domain reflects a jet spray burner configuration from work O'Loughlin and Masri [4]. The burner assembly, showed in figure 1, consists of the ultrasonic nebulizer device (5), which generates spray with specific SMD at the inlet of the central jet nozzle with a diameter of $d_j=4.6\text{mm}$. The spray at temperature 300K is carried downstream the central tube (1) by the co-flowing stream of air at the inlet (6). The annular co-flow assembly surrounds the central

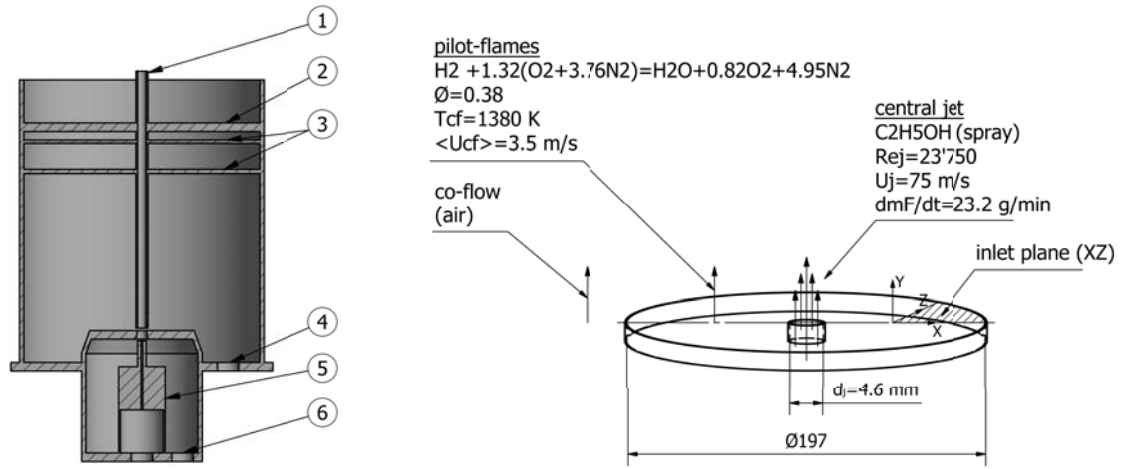


Figure 1. Half-section of the burner (left) and the inlet plane inset (right).

tube. Its diameter is equal to 197mm. The co-flowing mixture is fed in inlet (4), passes through the double glass beads (3) and terminates at the perforated plate (2) with 2200 holes, each with a diameter of 1.58mm. Lean hydrogen/air flames with specified temperature are issued from each of the hole with the velocity equal to 3.5m/s. Experimental data from several spray flames are available for different fuels, mass loadings and co-flow temperatures. As a reference for the current studies an ethanol spray flame is chosen for which the jet spray has bulk velocity of $U_j = 75$ m/s, the mass flow of liquid droplets is equal to 23.2g/min, the droplets $SMD = 40 \mu m$ and the co-flow temperature $T_{cf} = 1380$ K.

The simulation domain comprises of a rectangular volume segment of the burner and is aligned with the jet axis. It starts at the jet exit plane and extends $50d_j$ downstream. The radial dimensions of the domain are equal to $15d_j$. The domain is discretised by $312 \times 200 \times 200$ nodes compressed in the vicinity of the inlet plane and along the jet, i.e., in the region where high scalar gradients are expected. The resulting mesh spacings are as follow: $\Delta x = \Delta z = 1.9 \cdot 10^{-4} \div 1.0 \cdot 10^{-3}$ in the radial directions and $\Delta y = 2.1 \cdot 10^{-4} \div 1.7 \cdot 10^{-3}$ in the axial direction. Except the inlet and outlet, the boundary conditions applied in the simulations are characterised by the zero-gradient Neumann boundary condition. At the outlet the convective boundary condition is prescribed while at the inlet the experimental velocity profile is imposed. Outside the jet inlet region the hot vitiated co-flow of combustion products with temperature and velocity corresponding to the experiment is assumed. Instead of reproducing the exact droplet distribution issuing at multiple points from the jet nozzle the spray is injected from a single randomly picked point, which at each time step has different location. The droplets sizes follow the Rosin-Rammler distribution for which we define 10 classes of diameters with $SMD = 20, 40$ and $60 \mu m$. We analyse the flame behaviour depending on SMD and focus on its impact on both global and local flame features during the autoignition and propagation phases. Additionally we compare the lift-off height predictions (L_f) for three different co-flow temperatures $T_{cf} = 1270, 1330$ and 1380 K. We verify which parameter (SMD or T_{cf}) has bigger impact on it.

4. Results

4.1. Analysis of spatial and ILES resolutions

To assess the LES quality, the axial variations of resolution parameters based on calculated integral length scale l_0 and Kolmogorov length scale η_K are presented in figure 2. In a round jet, the integral length scale can be approximated by $l_0 \approx d_j (1 + B \cdot z)$ where $B \approx 0.09$ is the expansion rate of the jet [12]. Having the l_0 the Kolmogorov length scale can be computed as $\eta_K = l_0 Re_L^{-3/4}$, for which $Re_L = u' l_0 / \nu$ where the RMS of velocity u' is calculated as the spatial average value. The analysis of the ratio of the characteristic mesh spacings in the axial direction Δy across the whole domain shows that spacings between grid points were less than 45% of l_0 . At the same time they were not greater than $20\eta_K$ in most part of the domain. It seems that the used grid can be regarded as appropriate for ILES simulations.

The ILES assumptions hold for the perfectly stirred reactor (PSR) conditions, which correspond to the homogeneous sub-grid species and temperatures distributions inside the LES filter size Δ . To ensure PSR conditions the turbulent mixing should occur faster than the chemical reactions. The Damköhler (Da) can be viewed as an indicator of the PSR since Da decreases with decreasing Δ and it is defined as the ratio of subgrid time scale to the chemical time scale $Da_\Delta = \tau_\Delta / \tau_c = S_L / \delta_L \cdot \Delta / u_\Delta$ [3]. The sub-grid velocity fluctuations for Da calculations were estimated as $u_\Delta = \sqrt{2} / c_K \cdot \mu_{sgs} / \rho \Delta$ using computed sub-grid scale viscosity μ_{sgs} and taking the constant $c_K = 0.07$. The sub-grid viscosity was estimated applying the model of Vreman [13]. It is important to note that for PSR the $Da \ll 1$. However, one can note from figure 2 that there are spatial variations of Da substantially exceeding the value $Da = 1$. They are predominantly linked with the zones that are not resolved well, especially in the outer regions of the jet axis near to the inlet plane and also further downstream, where the grid spacings are bigger. On the other hand, upstream the jet in high heat release regions $Da \approx 5$ or even less. Even though this value is somewhat higher than the one assuring the ILES validity, the simulations still yield correct predictions of the experimental values of the lift-off height, as will be shown in the following subsections.

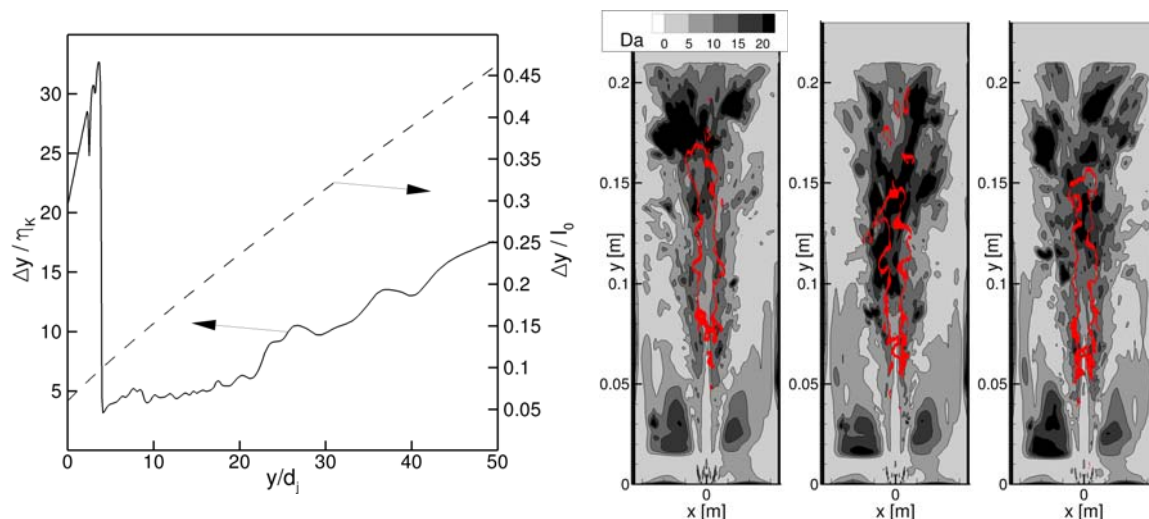


Figure 2. Axial variations of the grid resolution with respect to the characteristic flow scales (left image). Planar distributions of Da number with contours of the reaction zones for T_{cf} equal to: 1270, 1330, and 1380K (from left to right respectively).

4.2. Autoignition delays

Figure 3 shows the autoignition delay times reflected by means of the instantaneous maximum temperature growth. The presented results were obtained for each of the co-flow temperature and initial spray SMD. It can be seen that the autoignition occurs firstly and most rapidly for the smallest droplets (SMD=20 μm), regardless the co-flow temperature. The feature of spray with small initial SMD compared to higher SMD for constant fuel loading, is that the smaller one results in larger number of smaller droplets, increasing substantially the droplets surface. This determines the heat diffusion and evaporation rates. The differences in autoignition delays between different co-flow temperatures are the smallest for SMD=20 μm . The autoignition for intermediate droplets' SMD=40 μm appears almost at the same time instances, being only slightly delayed for low T_{cf} . Substantial differences in the temperature growth rate are evident only for the biggest droplets (SMD=60 μm). For the lowest T_{cf} =1270K the autoignition is delayed more than three times, compared with the results for T_{cf} =1380K. The instantaneous maximum fuel mass fraction growth rates for the smallest droplets' SMD for any of the T_{cf} , exceed the fuel growth rates of the other two cases by several times. The evaporation of the bigger droplets (SMD=40 and 60 μm) is rather slow and does not present such a substantial jump when the autoignition occurs. It can be seen that the autoignition delay is not directly related to the maximum fuel mass fraction, because the autoignition occurs in each case for completely different $Y_{F,max}$ and always below the stoichiometric mass fraction ($Y_{F,st} = 0.1$). The SMD is in this case the most influential parameter that affects the autoignition delay.

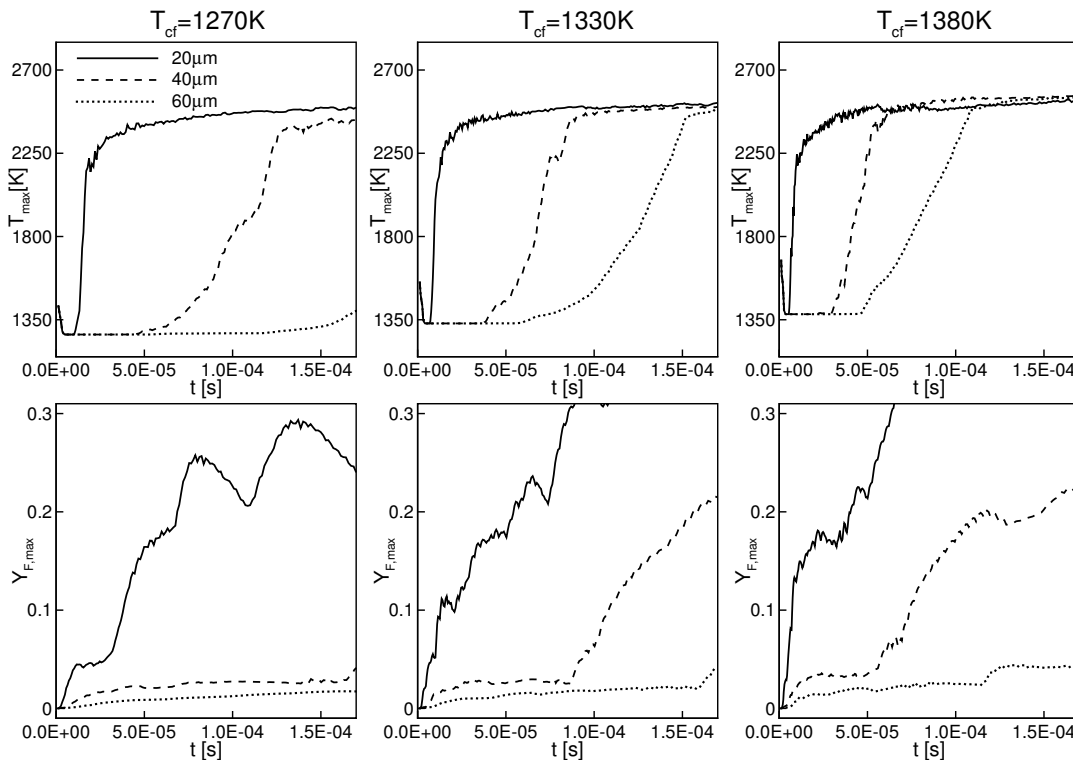


Figure 3. Evolution of maximum temperatures (upper row) and the gaseous fuel mass fractions (lower row) inside the domain.

4.3. Mean and instantaneous temperatures

Comparison of the lift-off heights prediction and the experimental flame depicted in figure 4 shows satisfactory agreement. The measured L_f in the experiment for $T_{cf}=1380\text{K}$ was reported as $L_f \approx 15$, similarly as the one obtained presently. Figure 5a) presents the instantaneous distributions of temperatures and the fuel mass fractions and figure 5b) shows the contours of heat release multiplied by the Takeno flame index for each T_{cf} with initial $\text{SMD}=40\mu\text{m}$. It can be seen that the lift-off height decreases due to increasing co-flow temperature. Inside the highest isotherm envelope there is a broad non-reacting fuel-rich region for the lowest T_{cf} . It is elongated mostly in the downstream direction. From the figure 5a) it is evident that the high temperature reaction zone slides upstream. This is due to the fact that some amount of fuel that evaporated from the spray core, mixes intensively with the oxidizer within the mixing layer that developed at the jet edge. The pockets of high heat release which forerun the autoignition are moved upstream and correspond to the lean fuel regions. However, due to small temperature, lowered by the heat diffusion from the hot co-flow into the spray core, the mixture ignites only further downstream. The Takeno flame index is defined as $\Upsilon = \nabla Y_{O_2} \cdot \nabla Y_{Fuel}$. It distinguishes the premixed combustion regime for which $\Upsilon > 0$ from the diffusion combustion where $\Upsilon < 0$. These correspond to the green and red regions, respectively, showed in figure 5b). The presented values of high heat release regions, multiplied by the Takeno index indicate the combustion mode within the reactive layer. The premixed regime region for the lowest T_{cf} is the smallest one and it extends downstream for increasing co-flow temperatures. The tip of each reaction zone is burning predominantly in the premixed mode while the unburnt fuel is further convected downstream where the combustion occurs mainly in the diffusion mode.

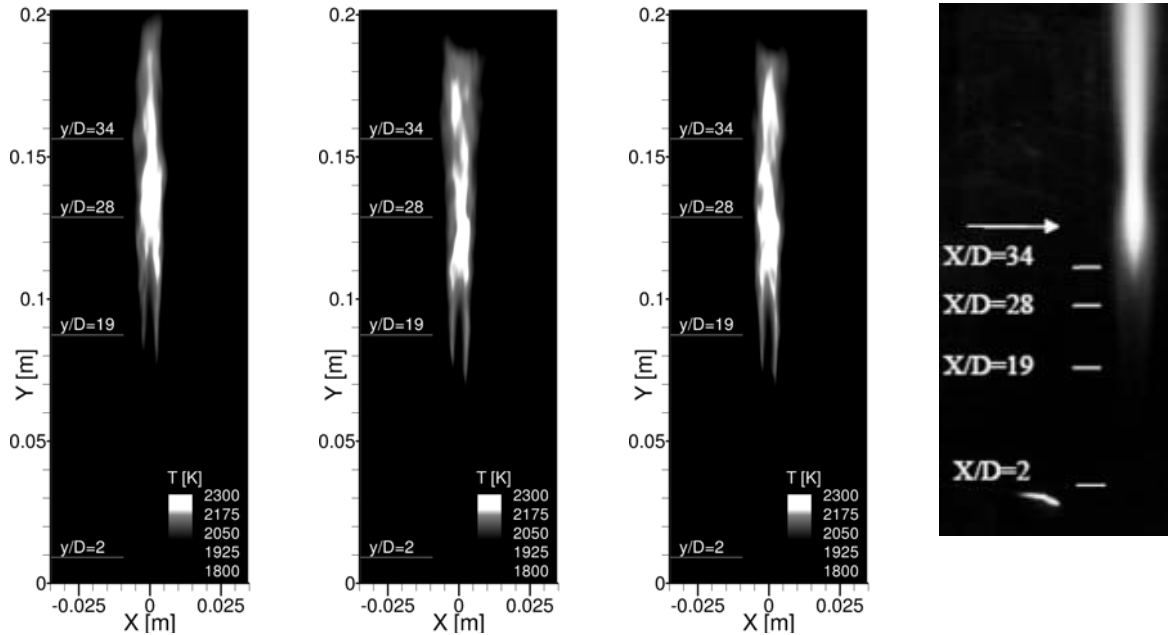


Figure 4. Mean temperature fields obtained for spray characterised by $\text{SMD}=40\mu\text{m}$ and different T_{cf} (from left to right): 1270, 1330 and 1380K. The last picture shows the experimental results with $T_{cf}=1380\text{K}$.

4.4. Droplet size distributions

Figure 6 shows the droplet size distributions at two distinct positions along the jet axis, i.e., $y/D = 28$ and $y/D = 19$. The bars with different colors denote different classes of the initial

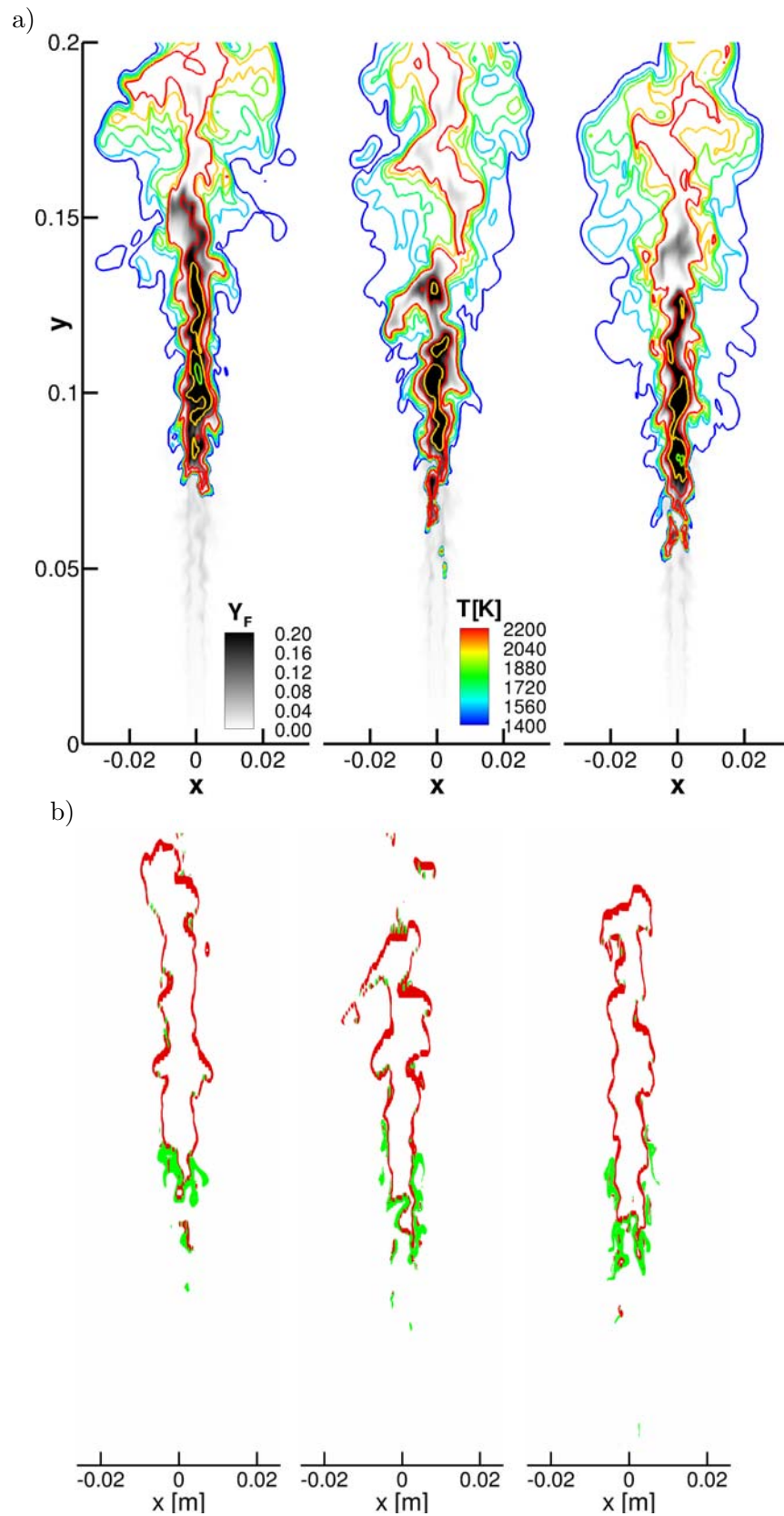


Figure 5. Instantaneous distributions of: a) temperatures (iso-lines) and fuel mass fraction (gray-scale field) and b) iso-contours of high heat release value multiplied by the Takeno index.

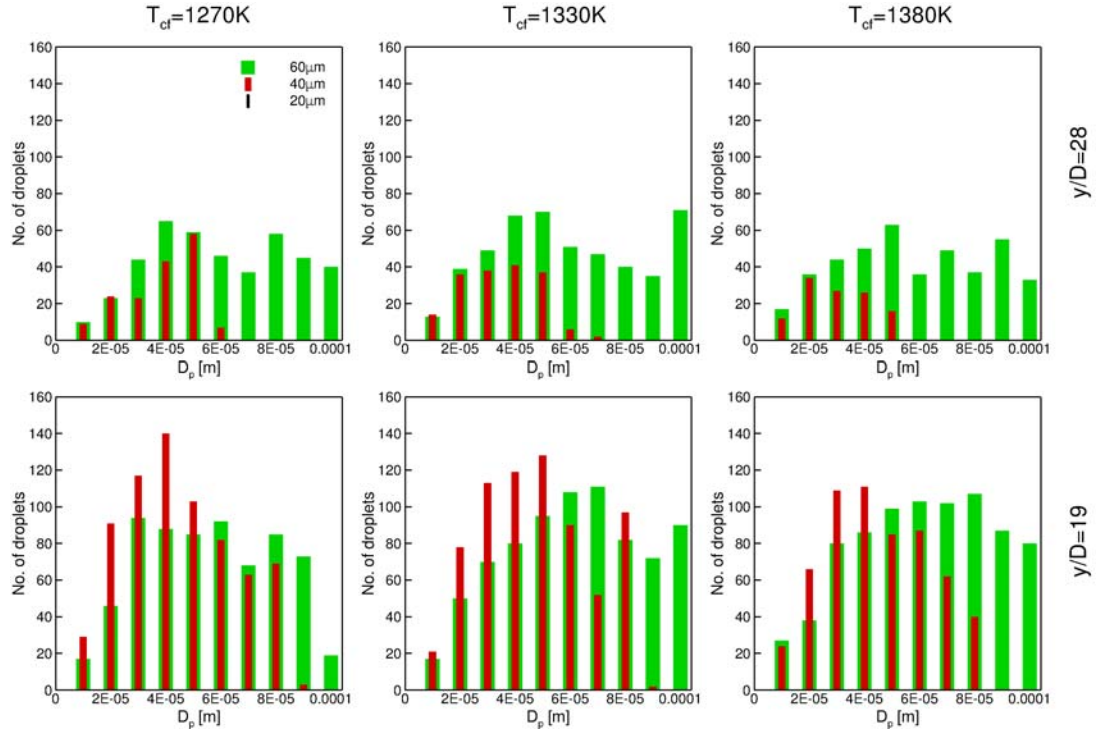


Figure 6. Spatial distributions of droplets for two axial positions of the jet: $y/D = 28$ (upper row) and $y/D = 19$ (lower row). Columns correspond to T_{cf} : 1270K (left), 1330K (middle) and 1380K (right).

SMDs. One may observe that droplets with the $SMD = 20 \mu m$ did not prevail to the downstream region and evaporated quickly. Concerning the impact of T_{cf} on droplets diameters one may observe that for its larger values the droplets evaporate quicker, as one could expect. This effect is well visible for droplets with $SMD = 40 \mu m$. In the case of spray with $SMD = 60 \mu m$ the influence of T_{cf} is less pronounced but still exists. It is interesting that in this case the total number of droplets in each of the classes is similar at different locations.

4.5. SMD impact

Instantaneous planar snapshots of temperatures distributions with the droplets represented by the spheres coloured by its temperature are presented in figure 7. Because small droplets evaporate quickly for the lowest $SMD = 20 \mu m$ the flame is attached to the injection nozzle. Significantly different behaviors are observed for the flames with higher SMDs. They are lifted and the lift-off height depends on SMD. Differences in the amount, size and temperature of the drops trapped within the reaction zone are evident. The bigger droplets ($SMD = 40$ and $60 \mu m$) prevail almost across the whole flame zone and are not fully consumed. It can be seen that for $SMD = 60 \mu m$ the flame is thinner and it is anchored further from the inlet ($L_f \approx 17D$ for $SMD = 60 \mu m$ and $L_f \approx 15D$ for $SMD = 40 \mu m$). One can also observe that in this case the number of droplets leaving the computational domain is much larger than in the simulations with $SMD = 40 \mu m$.

5. Conclusions

The current studies concerned the ILES analysis of influence of the co-flow temperatures and the spray size on the combustion process in spray jet flame. It was shown that the lift-off

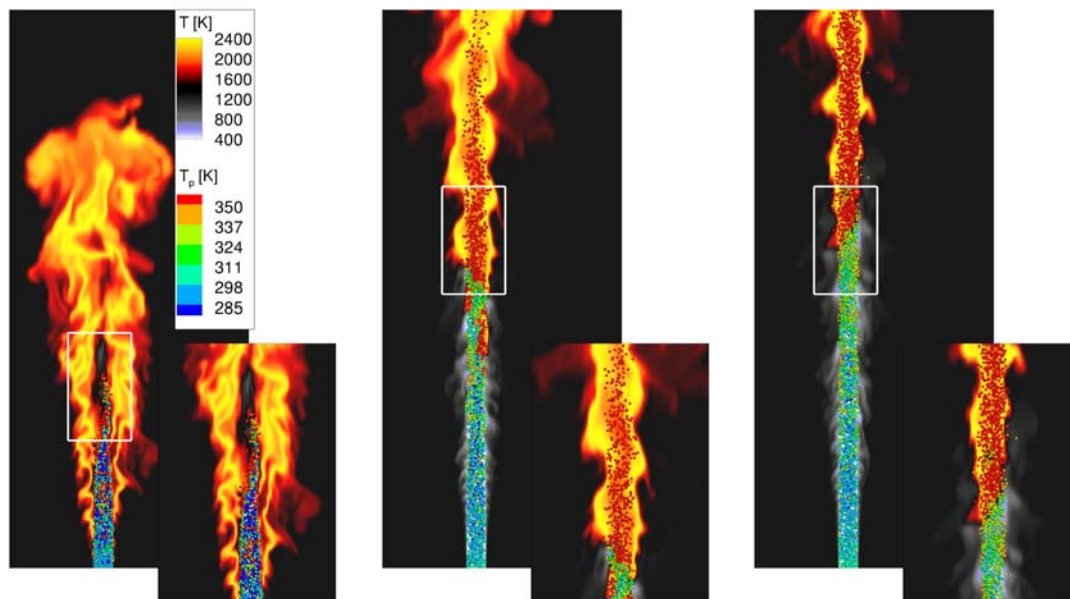


Figure 7. Instantaneous planar temperatures distributions for $T_{cf}=1380\text{K}$ and three different $\text{SMD}=20, 40$ and $60\mu\text{m}$. The droplets are coloured by its temperatures and scaled by the diameters. Insets show the tip of reaction zone.

height varies slightly with the co-flow temperatures. The co-flow temperature influences the flame by modifying the region of distinct combustion regimes, i.e., the volume of the premixed combustion mode increases with the increasing T_{cf} . The influence of droplet size turned out to be more pronounced than the co-flow temperature variations. Concerning the autoignition time the flame appeared earlier for smaller SMD values. This was connected to the fact that smaller droplets evaporated quicker and produced gaseous fuel more intensively. For the smallest droplets ($\text{SMD}=20\mu\text{m}$) the flame was attached, while for the cases with $\text{SMD}=40$ and $60\mu\text{m}$ it was lifted. It was observed that the lift-off heights were dependent on SMD and that this dependence was more pronounced than dependence on the co-flow temperature.

Acknowledgments

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