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MODELING ETHANOL SPRAY JET FLAME IN HOT-DILUTED COFLOW WITH TRANSPORTED PDF

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ABSTRACT

MILD Combustion, also known as flameless combustion, is attracting wide scientific interest due to its potential of high efficiency and low NOx emission. This paper focuses on the numerical modeling of one of the ethanol spray flame cases from the Delft Spray-in-Hot-Coflow (DSHC) burner, which has been used to study MILD oxidation of liquid fuels. The study has been carried out following the approach of dilute spray simulation. To properly account the turbulent two-phase flow system, a joint velocity-scalar PDF for continuous phase, and a joint PDF of droplet parameters for dispersed phase are employed respectively. Due to the high-dimensionality, the joint PDFs are solved by a Monte Carlo particle method, therefore it is refered to as 'Lagrangian-Lagrangian' approach. The evolution of gas phase composition is described by a Flamelet Generated Manifold (FGM) and the LMSE micro-mixing model. The droplet heating and evaporation processes are modeled with a parabolic temperature profile model. Validation of this modeling approach is carried out by comparison with experimental measurements. Results show that the spray behavior is successfully reproduced; the predicted droplet mean velocity components profiles for all droplet size classes are in very good agreement with the experimental data at various axial locations. Droplet Sauter Mean Diameter (SMD) have been accurately predicted. Gas phase velocity also matches well with experimental data. Gas phase temperature is in reasonable agreement with the experiment, however, it is under predicted at the near axis region. Improvement of the accuracy on temperature prediction can be made by using a non-adiabatic FGM table including an enthalpy variable.

***Keywords**: Spray combustion, MILD combustion, FGM, Transported PDF*

1. INTRODUCTION

Spray combustion is widely utilized in various engineering applications, such as industrial furnaces and propulsion systems. Modeling of turbulent spray combustion is particularly challenging, because many physical and chemical processes including turbulence, atomization, evaporation, combustion and radiative heat transfer are involved and interact with each other [1]. These phenomena and processes have to be modeled in a proper way in the sense that the main physical characteristics have to be accounted for but within a reasonable computational cost. For simplicity, many spray combustion studies have been carried out in the regime of dilute spray [2,3], and this is also the case for this study.

Transported PDF method proposed by Pope [4] has been proven to be a powerful closure method for modeling turbulent reactive flow. The most outstanding advantage of transported PDF method is that the mean reaction source term appears as a closed term. However, for the sake of reducing computation cost, the direct use of detailed chemistry is not employed in this study, instead the Flamelet Generated Manifold model proposed by van Oijen [5] is used. In FGM, the scalars, such as temperature, species mass fraction, density etc., are stored in the lookup table as a function of a few independent variables, e.g. mixture fraction and progress variable. The influence of turbulence is accounted for by the Probability Density Function (PDF) of the independent variables. The PDF for mixture fraction is often presumed as a beta function, and determined by the mean and variance value obtained during the turbulent combustion simulation. However, severial studies [1,6] already pointed out that due to the presence of droplet evaporation the beta shape PDF is no longer valid for mixture fraction in spray combustion. In transported PDF method, the PDF is directly solved, therefore the turbulence-chemistry interaction is considered in a more precise manner.

Moderate or intense low oxygen dilution (MILD) Combustion is a promising technology that mitigates the combustion-generated pollutants whilst meeting thermal efficiency needs [7,8]. Delft Spray-in-Hot-Coflow (DSHC) burner was designed to study the fundamental aspects of flameless oxidation of light oils [9]. The present paper reports a first numerical study of this flame with transported PDF method.

2. EXPERIMENTAL DADABASE

The schematic of the DSHC burner is shown in Figure 1. The hot-diluted coflow is produced by the secondary burner that operates on air and Dutch nature gas (DNG). This hot-diluted coflow is used to mimic the mixture of air with combustion products in MILD combustion furnace. The liquid fuel, ethanol in this study, is injected by a pressure swirl atomizer in the hot-diluted coflow.

The available experimental database includes the following data: radial profiles of coflow temperature, velocity components and O_2 volume concentration; radial profiles of the droplet diameter and velocity components at different axial locations; and radial profiles of gas phase temperature at different axial locations. A complete description on the DSHC burner and corresponding database can be found in [9]. These data are compared with the simulation results for validation purpose.

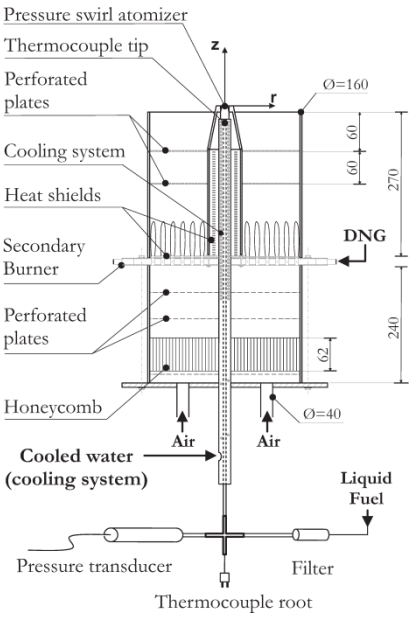

Figure 1. Schematic of DSHC burner.

3. NUMERICAL SETUP

3.1 Computation domain & boundary conditions

Figure 2 shows a picture of the DSHC flame, on which the computational domain of this study is illustrated with yellow rectangle. As the flame is axisymmetric, a 2D axisymmetric simulation is conducted. The inlet boundary is chosen such that it is sufficiently far from the atomizer tip to avoid the influence of the dense spray region and also below the region where the ignition starts. In this case, the axial location Z=8 mm is chosen as the inlet boundary, this is also the first axial location where the dispersed phase properties were measured.

The dispersed phase boundary conditions are assigned according to the corresponding experimental data. However, the gas phase boundary conditions cannot be directly specified from the measurements. This is because, firstly, the existence of the droplets prevents the use of Laser Doppler Anemometry (LDA) for gas phase velocity measurement in the spray region, therefore the gas phase velocity is obtained from the Phase Doppler Anemometry (PDA) measurements, assuming that the small droplets (D < 6 μm) strictly follow the gas phase behavior. However the PDA result only is available at a relative small region where the small droplets are present, and these data are insufficient to accurately assign the whole inlet boundary profiles. Secondly, as the FGM model is used as the combustion model, the control variables, mixture fraction and progress variable, have also to be assigned at the inlet boundary. But, they are not directly available from experimental measurement. However, the necessary properties are available at the coflow exit (Z = 0mm). A full spray combustion simulation including the spray atomization process is conducted with ANSYS Fluent15 to provide reliable boundary conditions at Z=8 mm for the present study. In the Fluent simulation, the pressure-swirl atomizer is modeled with Linearized Instability Sheet Atomization (LISA) model. The turbulence flow field is described by Reynolds Stress Model (RSM). And the turbulence-chemistry interaction, to be consistent with the current study, is also modeled by FGM model but with presumed shape PDF method. In this Fluent simulation, beta PDF is used for both mixture fraction and progress variable. To examine the reliability of the boundary condition provided by the Fluent simulation, not only the results at Z=8 mm but also at other axial locations are compared with experimental data. The compared variables include: the droplet velocity components for different droplet size classes, droplet Sauter Mean Diameter (SMD), gas phase velocity components as well as gas phase temperature. Reasonably good agreement with experimental data has been achieved by this Fluent simulation. The modeling detail and results of the Fluent simulation will be reported separately, part of the results can be found in [10]. This gives us enough confidence to employ Fluent simulation results as boundary conditions for the current study. The velocity, mixture fraction and progress variable boundary conditions for this study are shown in Figure 3.

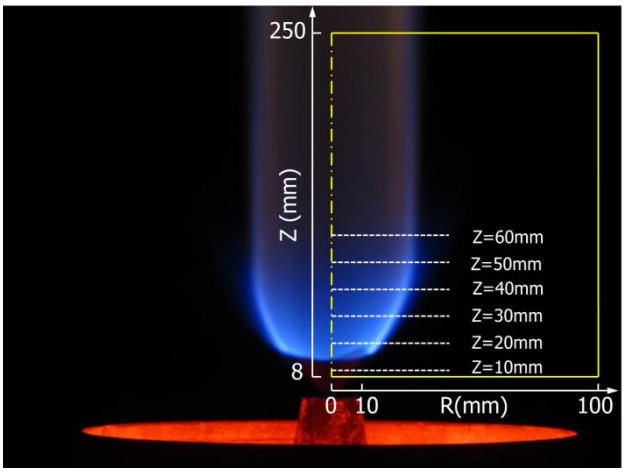

Figure 2 Picture of DSHC flame with indication of axial location of experimental data.

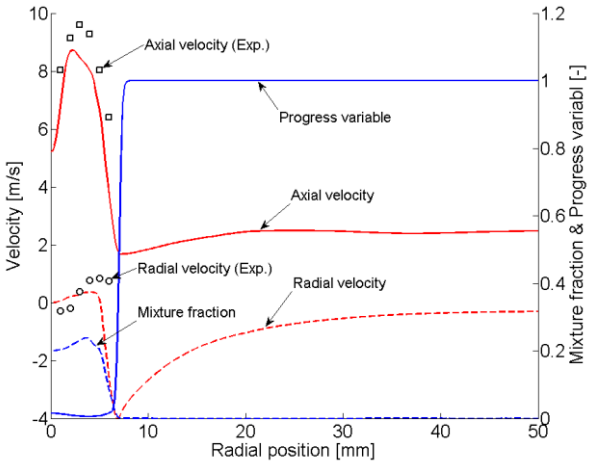

Figure 3 Boundary conditions for dilute spray simulation of the DSHC flame

3.2 Numerical model

The turbulent two phase flow system of the DSHC flame is described by a hybrid finite volume / transported PDF approach implemented in the in-house code 'PDFD'. The continuous phase is described by a joint velocity-scalar PDF, and the dispersed phase is described by a joint PDF of droplet position, velocity, temperature, diameter, and the gaseous properties 'seen' by the droplet. Due to the high-dimensionality, the joint PDFs are solved by Monte Carlo particle method. In contrast with more standard Eulerian-Lagrangian approach, in PDFD, both the gas phase and the dispersed phase evolution are defined by Lagrangian equations, therefore we refer it as 'Lagrangian-Lagrangian' approach. To overcome the bias error due to the limited number of computational particles in the Monte Carlo method, the mean velocities and Reynolds stresses are calculated using a Finite-Volume (FV) method, in which the Reynolds Averaged Navier Stokes (RANS) equations are solved. The algorithm of PDFD code is shown in Figure 4.

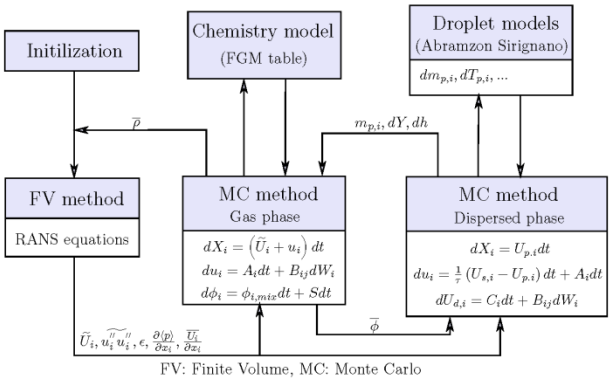

Figure 4 Schematic of the hybrid FV / MC algorithm in PDFD code

The finite volume submodel provides the mean velocity and its gradient, mean pressure gradient, Reynolds stresses and mean turbulent dissipation rate to the Monte Carlo part. The fluctuating velocity increment of gas phase particle is determined by generalized Langevin model (GLM), specifically, the Lagrangian isotropisation of production model (LIPM). To be consistent with LIPM, the isotropisation of production Reynolds-stress model (LRR-IPM), is used for the modeling of the pressure strain correlation in the finite volume part. The evolution of gas phase composition is described by FGM and the Linear Mean Square Estimation (LMSE) micro-mixing model [11], also known as interaction by exchange with the mean (IEM):

$$d\theta = \theta_{mix} + S\,d \tag{1}$$

$$\theta_{mix} = -\frac{1}{2}\omega_\theta\left(\theta - \tilde{\theta}\right)dt \tag{2}$$

Where ω_θ is the modeled scalar variance decay frequency. S is the source term. Since the tabulated chemistry model FGM is used, the scalar θ in this case include only the independent variables of the lookup table, namely, the mixture fraction and progress variable. Unlike the pure gaseous flame, the mixture fraction in spray combustion is no longer a conserved scalar, its source is due to the vaporization of droplets. The source term of progress variable is retrieved from the FGM lookup table as a function of independent variables, as shown in Figure 5. The influences of the spray are also represented by the extra source terms appearing in the momentum and Reynolds stress equations in the finite-volume, this is the so-called 'two-way coupling'.

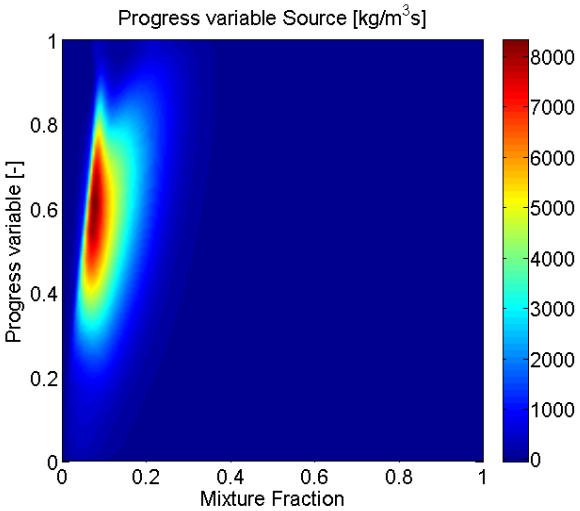

Figure 5 Source term of progress variable

The droplet heating and evaporation processes are modeled with the 'parabolic temperature profile model' which is in the category of finite conductivity models. In contrast with the widely used infinite conductivity model, where the temperature distribution inside the droplet is assumed uniform, this model takes into account the finite rate heat conduction inside the droplet. This is important where the droplet heating process is fast as is the case in the hot-diluted coflow condition of this study.

In flamelet-like models, the multi-dimension flames are considered to be a set of 1D flamelets. The 1D flamelets are characterized by different controlling parameters to describe the local variations of the real flame. For the FGM model, the controlling parameters are mixture fraction and progress variable. There are different methods existing for the construction of the 2D FGM lookup table [5]. A commonly used one is to first calculating different steady flamelet equations with scalar dissipation rate increasing from a zero to the extinction value. And then mapping these steady flamelets together with the unsteady flamelet at the extinction scalar dissipation rate to mixture fraction and progress variable space. Another approach is to solve the unsteady process of 1D diffusion flame in physical space from pure mixing until the steady flame is established. The flamelets at different time are then transformed into mixture fraction and progress variable space. Comparing to the "extinguishing" FGM generated by the first method, the second method generates a "auto-igniting" FGM table. Therefore it is more suitable to describe the auto-ignition process of the DSHC flame. The auto-igniting FGM table in this study is generated with the CHEM1D code developed at the Eindhoven University of Technology [12]. The detailed ethanol high temperature

oxidation mechanism containing 57 species and 383 reactions by Marinov [13] is employed. The ignition process is illustrated by the temperature profiles in mixture fraction space with increasing time, as shown in Figure 6. The progress variable in this study is defined as:

$$C = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{H_2O}}{M_{H_2O}} + \frac{Y_{H_2}}{M_{H_2}} \quad (3)$$

Where Y and M denote the mass fraction and molecular weight.

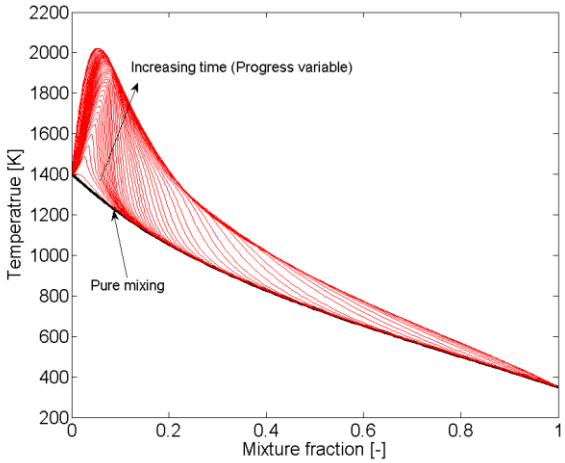

Figure 6 Temperature profiles for auto-ignition FGM table

3. RESULTS AND DISCUSSION

3.1 Dispersion phase results

In spray combustion, the dispersed phase not only provides the evaporated fuel vapor for combustion, but also directly modulates the continuous phase flow field. A correct prediction of the dispersed phase behavior is essential for successful modeling of spray combustion. Therefore the predicted droplet results are firstly presented and compared with the experimental data to validate the dispersed phase sub-models. The gas phase results will be discussed in next subsection.

Droplet mean axial and radial velocity profiles are shown in Figure 7. The results are plotted in a matrix of subplots with each subplot representing a certain droplet size class (columns) at a certain axial location (rows). To save space, only five droplet classes are shown here. The droplet size increases from left to right of the matrix and the axial location increases from bottom to top. It can be clearly seen that the predicted droplet velocity matches very well with the experimental for all droplet classes at all the axial locations compared. At higher axial location, the simulation results have a wider radial distribution than the corresponding measured data. This is because in the experiment, the PDA measurement is only carried out in the region where the droplet concentration is relatively high. At the inner and outer spray edge where the droplet number density is low, the experimental data is not available.

Droplet Sauter Mean Diameter (SMD) is shown in Figure 8. In the region where the experimental data are available, both the trend and magnitude of SMD are correctly predicted. The slight under-prediction at the spray outer edge (large radial position) may be attributed to the inaccurate specification of droplet size distribution at the inlet boundary. In this simulation, droplet are considered only in the diameter range of [0, 70] μm, respecting the known total mass flux. This was done because the number density of the droplets larger than 70 μm is quite low in this flame, due to both the quick evaporation and changed atomization mechanism by the hot coflow as presented in the experimental paper by Rodrigues et al [9]. However, exclusion of the big droplets may have a non-negligible influence on the mass flux of large droplet at the spray outer edge because of their ballistic trajectories and the large amount of mass they contain.

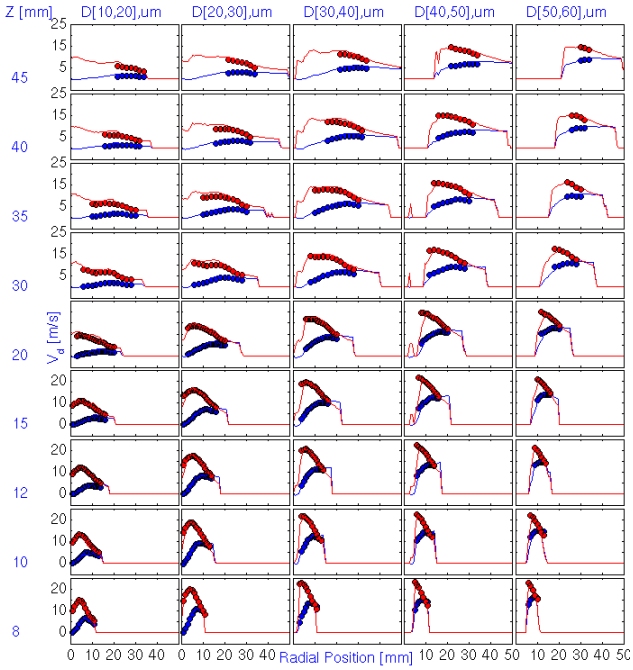

Figure 7 Droplet velocity: solid lines - simulation results, circular dots - experimental data, red - axial velocity, blue - axial velocity.

3.2 Gas phase results

From flame picture Figure 2, it can be clearly observed that the DHSC flame is a lifted flame. Since the spray is issued into a hot-diluted coflow which temperature much higher than the auto-ignition temperature of ethanol, the spray flame is mainly stabilized by the growth of auto-ignition kernels. The lift-off height is therefore a balance between the auto-ignition delay time, the evaporation time scale and the flow time scale. As demonstrated in [10], the steady flamelet model is unable to predict the lift-off nature of this flame, and therefore leads to a wrong prediction of the flame structure. However, the auto-ignition FGM model used in this study, can capture the flame lift-off. Although there is no quantitative measurement on the lift-off height of this flame, by comparing flame picture Figure 2 and OH concentration and temperature field in Figure 10, we could conclude that the flame lift-off has been rather accurately predicted.

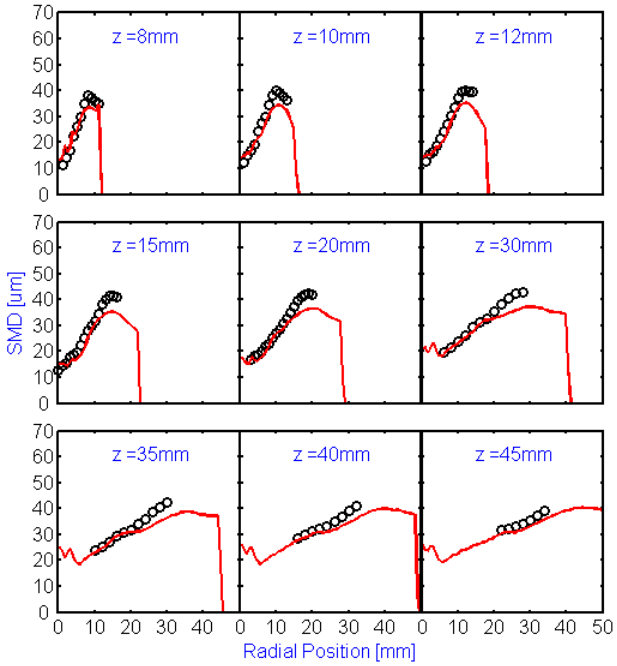

Figure 8 Droplet Sauter Mean Diameter: solid lines – simulation results, circular dots – experimental data.

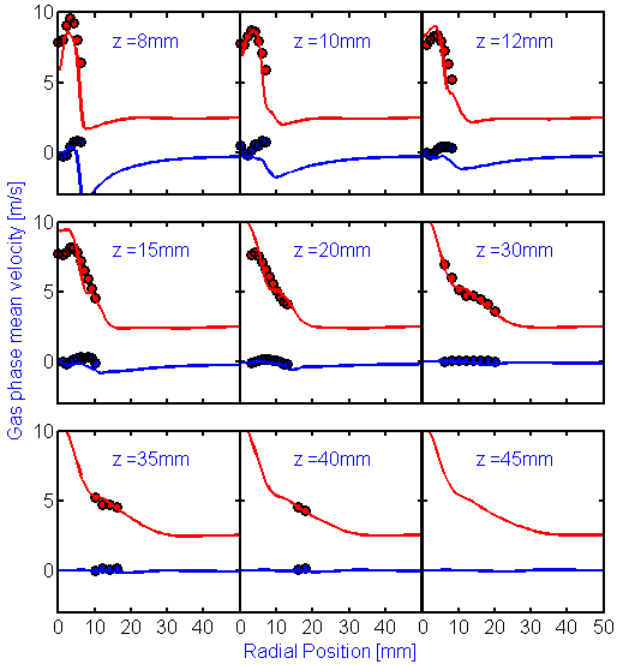

Figure 9 Gas phase velocity: solid lines - simulation results, circular dots - experimental data, red - axial velocity, blue - axial velocity.

Gas phase velocity and temperature are shown in Figure 9 and Figure 11 respectively. Good agreement with the available measurement data is observed for both mean axial and radial velocity profiles at all the axial locations compared. A slight under-prediction of the gas phase radial velocity at the lower axial locations can be explained from the following two aspects: first, the gas phase velocity boundary conditions obtained from Fluent simulation have some discrepancies with the experimental data, as shown in Figure 3. The reason for these discrepancies are explained in [10]. Second, the experimental gas phase velocity is obtained by PDA with small droplets as tracer. The small droplets need time to fully follow the gas phase, therefore the PDA results at the lower axial location maybe cannot been exactly interpreted as gas phase velocity. Further downstream, where the PDA tracer fully followed the gas phase flow, the match between the simulation and experiment becomes better. From axial location Z=45 mm onward, not enough tracer droplets are available due to the evaporation, therefore no experimental data are available thereafter.

The gas phase temperature in the spray region has been measured with Coherent Anti-Stokes Raman Scattering (CARS) technique for spray combustion [9]. A reasonable good agreement with the experimental data is obtained in this study. The flame peak temperature as well as the flame width are correctly predicted. The radial position of the peak temperature is a little shifted towards the center. This may mainly be caused by the mixture fraction profile specified at the inlet boundary. As explained in [10], the Fluent simulation used for providing inlet boundary information predicts smaller spray dispersion angle comparing with experiment. Consequently the distribution of the vaporized vapor is also narrower than that in reality. Close to the spray axis, an opposite temperature trend is predicted. The simulation shows a small temperature peak in the center, while the temperature progressively decreases toward the center in the experiment. This is because near the spray axis many small droplets exist, considerable gas phase enthalpy loss happens due to the fast evaporation of small droplets. The enthalpy loss, however, cannot be accounted by the 2D adiabatic FGM table used in the current study. As a consequence, the temperature has been over-predicted in this region. This problem can be solved by including enthalpy loss as another independent variable of the FGM table, namely, using a non-adiabatic FGM table.

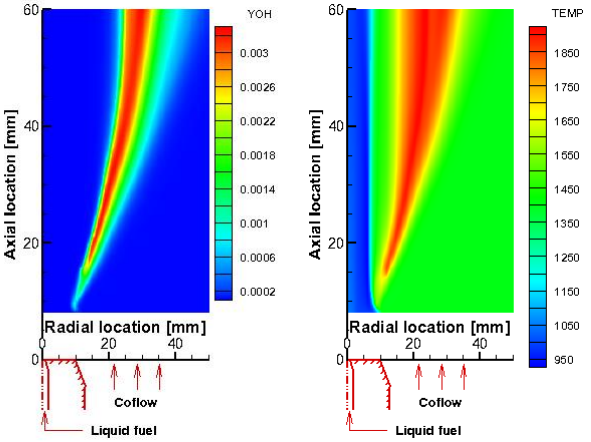

Figure 10 Contour plots from simulation results, left: OH mass fraction, right: gas phase temperature.

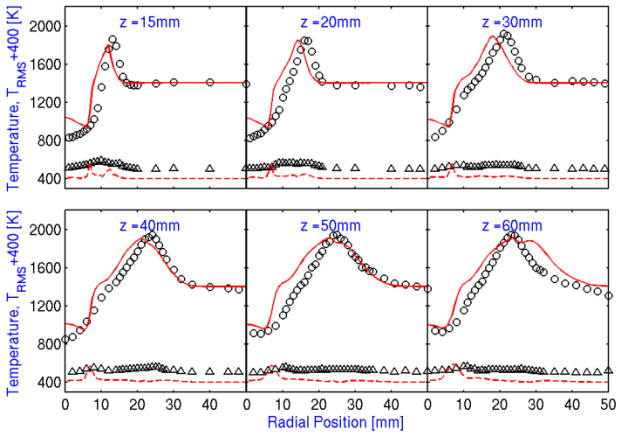

Figure 11 Gas phase mean and RMS temperature: solid line – mean temperature simulation , dashed line – RMS temperature simulation, circular dots - mean temperature experiment, triangular dots – RMS temperature experiment.

4. CONCLUSIONS

In this paper, we reported a first numerical investigation of Delft Spray-in-Hot-Coflow flame with transported PDF method and FGM model. The in-house hybrid finite-volume/transported PDF code "PDFD" is used for the simulation. The mean gas phase flow field is calculated by the finite volume part with Reynolds Stress turbulence model. The gas phase fluctuation, the turbulence-chemistry interaction as well as the droplet evolution are represented in the Monte Carlo part. These two parts are coupled in the way that the finite volume part provides the gas mean properties that are required for the Monte Carlo part calculation, and the latter one feeds back the gas phase density to the finite volume part. The continuous phase is described by a joint velocity-scalar PDF, and the dispersed phase is described by a joint PDF of droplet position, velocity, temperature, diameter, and the gaseous properties 'seen' by the droplet. A ‘parabolic temperature profile model’ is used to describe the droplet heating and evaporation processes.

The current modeling approach is validated by comparing the predicted droplet and gas phase properties with available experimental data. In general, very good agreement is obtained. Droplet velocity, Sauter Mean Diameter are all in good agreement with measured data, showing that the spray sub-models including the evaporation and dispersion models used in this study are suitable for modeling the DSHC flame. The lift-off characteristics of this flame have been correctly captured by the auto-ignition FGM momdel used in this study. Gas phase velocity also matches very well with the available experimental data. Gas phase temperatrue are in reasonable agreement with experimental data, showing the capability of the current modeling approach. However, it is also realized that the 2D adiabatic FGM table used in this study is insufficient to account the enthalpy loss due to the droplet evaporation, which resulted in a over-prediction of the gas phas temperature at the near axis region.

5. ACKNOWLEDGEMENT

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