Application of the FGM Method to Spray A Conditions of the ECN database

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Abstract

Modeling turbulent diesel spray combustion which combines complex flow and transport phenomena with combustion event including a vast amount of species and reactions is a major challenge. The Flamelet Generated Manifold (FGM) method is a promising technique to model reacting flows using tabulated chemistry approach. The method is adopted for diesel spray combustion by tabulating chemistry as a function of the mixture fraction (Z) and a reaction progress variable ($\mathcal{Y}$). In previous work, the method has been successfully applied to simulate Spray H cases as defined by the engine combustion network (ECN). Two different tabulation approaches (igniting counterflow diffusion flames (ICDF) and homogeneous reactors (HR)) were investigated and compared to the available experimental data of the ECN.

In this paper, the FGM method is applied to simulate Spray A conditions of the ECN. First, the sensitivity of the spray sub-models (atomization and breakup models) is studied for the non-reacting case of the Spray A setup. Later, the FGM approach is applied on the reacting case for FGM's generated with two different n-Dodecane reaction mechanisms, using two tabulation approaches, and with and without inclusion of a turbulent closure (PDF approach based on variance of Z). The 3D-RANS (Reynolds Averaged Navier-Stokes) simulations are performed with the commercial CFD code STAR-CD. The combustion results are analyzed by comparing the simulated and measured ignition delays and lift-off lengths. One mechanism results in ignition for all simulations, whereas the other mechanism does not. It was found that this can be attributed to the different sensitivity of the mechanisms to the strain rate. In general, HR tabulation predicts shorter ignition delay and lift-off length (LOL) than the ICDF in line with the observations from previous work. The atomization model does not show major effect on ignition delay however it affects the LOL significantly in both tabulation approaches. Inclusion of the turbulent closure does not affect ignition delay or LOL predictions. In general compared to the experiments, the ICDFs slightly over predict whereas the HRs systematically under-predicts.

Introduction

Diesel spray combustion includes complex and heterogeneous processes, majorly atomization, evaporation of a dense liquid spray, and a subsequent combustion event in a turbulent flow environment. These processes are nonlinear and controlled by multiphase, diffusion and species transport phenomena. Modeling the interaction between those complex phenomena poses a huge challenge to the research community. Efficient numerical models could greatly reduce the time and cost involved in engine and engine related studies. A wide range of numerical models and sub-models exist in literature [1-6] by various research groups which are inherently different in many aspects. Unfortunately, well-documented and validated experimental data is scarce. For that reason the Engine Combustion Network (ECN) motivated to generate a standard experimental database [7] at engine-like conditions, explicitly for the validation of computational models. The engine research team of the Combustion Technology (CT) group at Eindhoven University of Technology (TU/e) is contributing to this network by both experimental and numerical work.

The Flamelet Generated Manifold (FGM) method is one of the promising tabulated chemistry based methods [8, 10] to model turbulent reacting flows. The FGM method, in nutshell, combines advantages of (i) the laminar flamelet concept [11] which assumes that turbulent flame can be considered as an ensemble of laminar flamelets since the chemical reactions timescale are significantly less than the turbulent timescales and hence the reaction zone are not disturbed by turbulent eddies; and (ii) the Intrinsic Low Dimensional Manifold (ILDM) approach [12], where the chemistry system is reduced by tabulating chemistry as a function of control variables. In recent years, the FGM method has been extended to model igniting diesel spray characteristics (ignition delay and flame lift-off length) in diesel engine conditions [13, 14]. Canonical igniting systems are preprocessed and tabulated as function of two control variables, Mixture Fraction (Z) and Progress Variable ($\mathcal{Y}$), to track mixing and reaction progress. Previously, the method was applied successfully to predict the ignition behavior as func-

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tion of ambient gas O_2-concentration and temperature for the baseline *n*-heptane (Spray H) cases of ECN. Also the effect of two different chemistry tabulation methods Igniting Counter flow Diffusion Flames (ICDFs) and Homogeneous Reactors (HRs) was included [14].

In the present work, the method is further applied to simulate spray A of ECN since that it is with a new surrogate fuel *n*-dodecane which is closer to diesel. The aim is to obtain a benchmark model by investigating model sensitivities and new mechanisms which are still in development. RANS (Reynolds Averaged Navier-Stokes) based numerical simulations are performed using the STAR-CD Computational Fluid Dynamics (CFD) package. The model settings that have been used in the earlier study [14] are adopted in this study as the ambient conditions are same for Spray A & Spray H. However, in the current study, a more extensive spray study is carried out to assess the difference between the different sub-models available. This is explained in the 'Spray Modeling' section of this paper. The optimum spray models are chosen to simulate the combustion event using FGM. In further sub-sections of the paper the FGM method for two tabulation approaches is described briefly. The results are compared to with measurements and discussed in the results section.

Spray modeling

Accurate spray modeling is a crucial requirement to model the combustion event in a more reliable way. In the previous study [14], the Lagrangian spray model study is made with respect to turbulence models and numerical parameters like time step and grid size. Now with these optimized settings a sensitivity study is performed with respect to the available spray sub-models in STAR-CD for atomization and droplet break-up. The available models in STAR-CD are shown in Table 1.

Table 1: Spray sub-models in STAR-CD.

| **Droplet Break-up Models**	**Atomization Models**
Reitz and Diwakar [15]	Huh [18]
Pilch and Erdman [16]	Reitz and Diwakar [15]
Hsiang and Faeth [17]	MPI [19]
	Modified MPI [20]

Atomization models differ in the way droplet size distribution and initial velocities are calculated. The difference between the droplet break-up models is the correlations that are used to estimate the time scale of the break-up process and the stable droplet diameter. The only precondition of using these sub-models is that the Reitz and Diwakar atomization model has to be used in conjunction with the Reitz and Diwakar droplet break-up model. It should be noted that no constant/coefficient in any of the sub-models is tuned, so the simulations are performed with the default settings.

The models are applied for the non-reacting case of Spray A. The comparison will be made based on the vapour penetration length and the liquid length results. Here, the spray penetration length is defined as the farthest point from the nozzle exit where mixture fraction is over 0.001%, and liquid length is defined where void fraction exceeds 0.15%. The operating conditions and the model settings are presented in Table 2.

Table 2: Operating conditions and model settings.

Fuel	*n-dodecane*
Injection rate (g/s)	~2.40
Injection duration (s)	1.5e-3
Nozzle hole diameter (m)	90e-6
Fuel temperature (K)	363
Ambient temperature (K)	900
Ambient density (kg/m3)	22.8
O_2 [vol%]	0 - 15
Grid type	3D, uniform
Cell width (m)	0.25e-3
Time step (s)	1e-6
k-ε turbulence model	Standard high *Re*
Nozzle flow model	Modified MPI [20]
Collision model	O'Rourke [21]

First, vapour penetration results are compared. The representation for each model is *RD* (Reitz and Diwakar), *PE* (Pilch and Erdman), *HF* (Hsiang and Faeth), *HUH* (Huh), *MPI* (MPI) and *MPI2* (Modified MPI).The general trend of spray models is similar. To avoid confusion in Figure 1, only the best cases are presented. The closest match with experiments is obtained with the *MPI* atomization model. In addition to *MPI*, the combination of *MPI2* and *RD* models predicts the penetration accurately until $t \sim= 0.4$ ms. This is important since the ignition for the reacting case occurs around this time in the experiments ($t_{ID} = 0.4$ ms). For the rest of the cases, there is an over-prediction of the spray length during the early stages. After $t \sim= 0.5$ ms, an under-prediction starts for all available models [22].
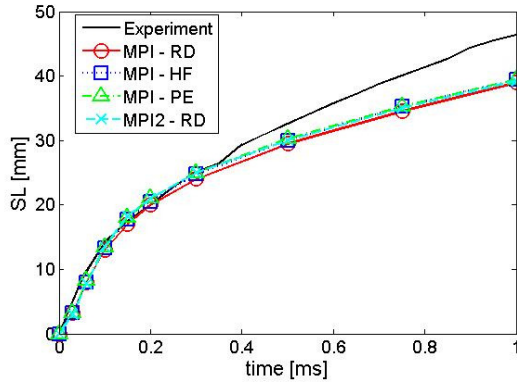
Figure 1: Vapor penetration as a function of time for *MPI-RD* (red), *MPI-HF* (blue), *MPI-PE* (green), *MPI2-RD* (cyan).
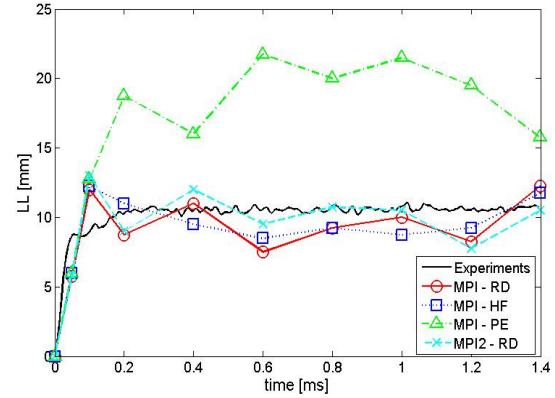
Figure 2: Liquid penetration as a function of time for *MPI-RD* (red), *MPI-HF* (blue), *MPI-PE* (green), *MPI2-RD* (cyan).

For the combination that performed well in the vapor penetration study the liquid length is analyzed in more detail. From Figure 2 a drastic deviation from the experimental values is observed for the *MPI-PE* combination. All other cases perform equally well. The main difference between simulations and measurement is the slight decrease in liquid length after reaching the maximum value. This phenomenon is not observed in the experimental results. More investigation is required to explain this discrepancy. However after $t \sim= 0.2$ ms, the predicted liquid lengths approach the experimental data with an acceptable degree.

In the previous study [14], the *RD-RD* combination was used as the spray model. Here, it will still be applied as the reference point. In addition to that, the combination of *MPI* atomization and *RD* droplet break-up models is selected based on the current study.

FGM method- reacting flow modeling

The general methodology of FGM, used in this work, consists of two major parts: one is pre-tabulation of detailed chemistry and the other is coupling this database (as look-up form) with turbulent flow calculations in a CFD solver. The interaction is depicted in Figure 3. The look-up variables and their variances are additional scalar transport equations [23] which are solved in STAR-CD simulations, next to mass- and momentum-conservation equations. The source term from droplet evaporation in STAR-CD acts as a source to mixture fraction (Z). However, in this method, the direct influence of the droplet evaporation on flame structure is neglected since, in these spray applications, the droplets evaporates at a shorter length compared to the ignition location. The source term of the progress variable and its variance, and the temperature are retrieved from the database using the lookup variables (transported in the CFD solver) at each time step.
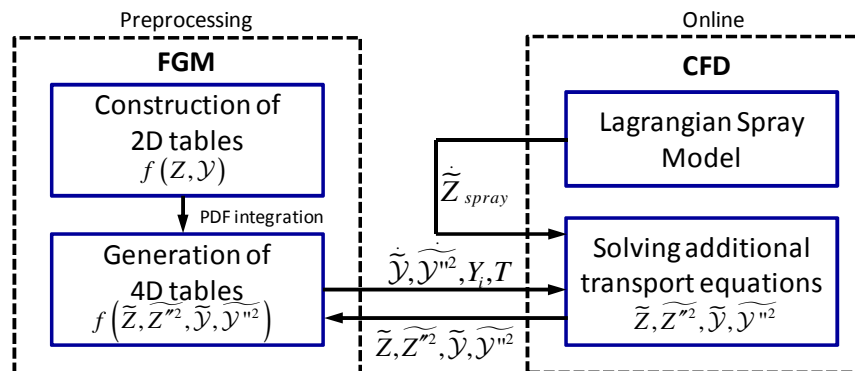

Figure 3: Interaction of CFD-FGM in STAR-CD

Two different approaches are employed independently to generate chemistry tables.Then the tables are integrated to enable turbulent closure of the chemical source terms. Further details are furnished in the following sections.

Generation of the database

Two canonical systems have been defined to generate the databases for igniting systems being Igniting Counter flow Diffusion Flames (ICDF) and Homogeneous Reactors (HR). In the ICDF approach a set of one-dimensional laminar flames are solved with CHEM1D (in-house code) [24]. The schematic of the counter flow diffusion flame in CHEM1D is as shown in Figure 4. To represent the non-premixed nature of diesel combustion, oxidizer and fuel streams are considered as two opposing streams which move towards each other and react at a plane close to the stochiometric region. The set of governing equations [25] which describes counter flow diffusion flames are solved, for both igniting and stationary to cover the entire regime of diesel combustion. Ambient conditions and boundary conditions for temperature and composition at either side, follow directly from Table 2. The igniting flames are obtained by solving time dependent solution starting from an adiabatic mixing frozen state solution at one strain rate of $500 \ s^{-1}$. The solutions are tracked in time to capture the auto-ignition process until a steady state is reached. The composition is augmented by a series of stationary flames with different strain rates starting from $500 \ s^{-1}$ and decreasing to a value $1.0 \ s^{-1}$. The low strain rate solutions approach towards a chemical equilibrium state. The influence of the strain rate on the FGM tables is explained in detail in [26].
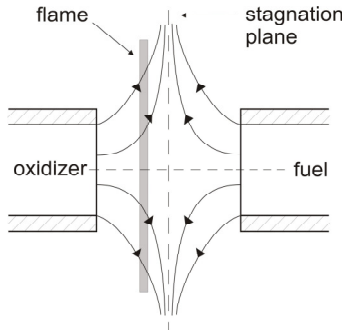
Figure 4: Schematic of counterflow diffusion flame setup.
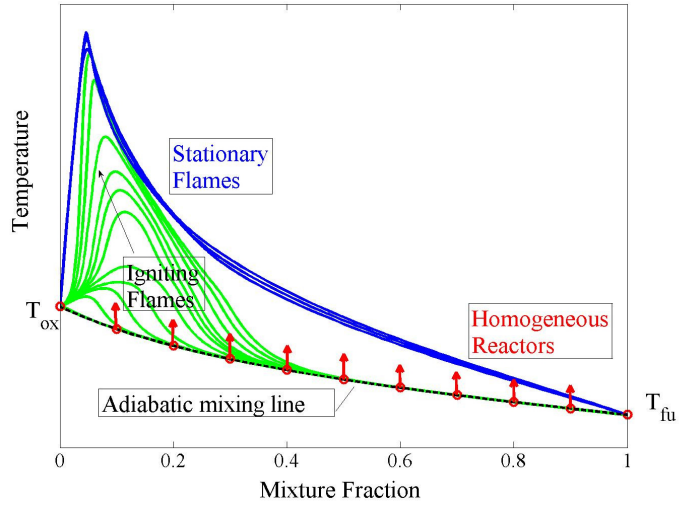
Figure 5: Illustration of mixing line, HRs, ICDFs.

The detailed chemistry solutions (of igniting and stationary flames) are obtained in time and spatial coordinates. These coordinates are transformed into two control variables i.e. mixture fraction (Z) and progress variable $(\mathcal{Y})$. The mixture fraction definition is adopted from Bilger [27]. The progress variable $(\mathcal{Y})$ is defined based on two requirements, i.e., it has to monotonically increase with reaction progress and it has to represent various stages of the combustion event adequately. In this study, weighted mass fractions of carbon dioxide (CO_2), carbon monoxide (CO) and hydroperoxyl (HO_2) are chosen:

$$\mathcal{Y} = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{HO_2}}{M_{HO_2}} \tag{1}$$

2D laminar tables are constructed using ICDFs chemistry data, based on two control variables with 101 points in each dimension.

In the HR approach this 2D manifold is generated using homogenous reactors, i.e. simplified zero-dimensional reactive systems. Here, the system does not consider diffusion and transport phenomenon during reactions, which is a fundamental difference from ICDFs. A complete series of HRs are computed that together span the same range in mixture fraction as defined by the adiabatic mixing line for the ICDF database as shown in Figure 5. A set of simulations from $Z = 0$ (pure oxidizer) till $Z = 1$ (pure fuel) is carried out to tabulate in

the entire mixture fraction space, in a discrete manner. Then again, 2D laminar tables are constructed with the table resolution of 101 points in each dimension.

Probability Density Function (PDF) integration

The effect of turbulence on chemistry is taken into account by a presumed PDF approach. The quantities in the 2D table are integrated with a β-PDF that is a function of the means and variances of the two control variables. When Z and $\mathcal{Y}$ are assumed statistically independent, the mean quantities are defined as,

$$\tilde{f} = \int\limits_0^1 \int\limits_0^1 f(Z,\mathcal{Y})P(Z\|\tilde{Z},\widetilde{Z''^2})P(\mathcal{Y}\|\tilde{\mathcal{Y}},\widetilde{\mathcal{Y}''^2})dZd\mathcal{Y} \tag{2}$$

After β-PDF integration, a 4D table is obtained. More details about the implementation of β-PDF integration on FGM can be found in [14]. In this work, only the fluctuation of mixture fraction is used to close chemical source terms; for now the fluctuation of the progress variable is omitted in the PDF integration. Tables with and without $\widetilde{Z''^2}$ (9 discretization points) are considered to evaluate the effect of $\widetilde{Z''^2}$. 101 points in Z and 9 points in $\widetilde{Z''^2}$ are used.

n-Dodecane reaction mechanisms

Currently the ECN group aimed at developing reduced reaction mechanisms for n-dodecane combustion. Here, two different reaction mechanisms are used to generate the chemistry database. One is the mechanism from Krithika and Pitsch (consisting of 253 species and 1437 reactions) [28], and the other is from Som et al. (consisting of 124 species and 476 reactions) [29].These mechanisms are referred in this paper as Krithika, Som respectively.

Combustion results and discussion

Reacting flow simulations have been performed in STAR-CD using FGM tables. The ignition characteristics resulting from the simulations are compared with Spray A measurements of ECN.

The ignition delay is one of the characteristics that quantify the time when ignition has started. It is defined as the time taken to reach the temperature, in any cell of the domain, which is half the rise to the maximum temperature that it could reach from initial value of 900 K. The pressure based ignition delay definition (as used in experiments) is not feasible because not the entire combustion chamber is considered for the modeling. All ignition delay predictions from the simulations using FGM are shown in Table 3. It is observed that with Krithika mechanism the ignition delay is slightly over-predicted with the ICDF approach, whereas it is under-predicted with the HR approach. This is due to the higher source terms for $\mathcal{Y}$ in HRs compared to ICDFs. A similar trend was observed in earlier work and the possible reasons were explained in [14]. The change of the atomization model from *RD* to *MPI* does not show a significant effect on the ignition delay results, for both of the tabulation approaches. This might be due to the reason that the source $\mathcal{Y}$ has not much effected due to atomization model change, although mixture composition effected. In both the tabulation approaches, inclusion of $\widetilde{Z''^2}$ doesn't affect the ignition delay. Although the temperature and species fields show differences, these are not reflected in the ignition delay since the ignition delay is based on maximum temperature in the domain.

Table 3: Ignition delay results from simulations, comparison with experimental value.

Method	ICDFs		HRs	
Tables \ Mechanism	**Krithika**	**Som**	**Krithika**	**Som**
101X101_RD-RD	*0.49*	*-- (No ignition)*	*0.32*	*0.21*
101X101_RD-MPI	*0.51*	*0,59*	*0.31*	*0.22*
101X9X101X1_RD-RD	*0.50*	*-- (No ignition)*	*0,31*	*-- (No ignition)*
Experimental (Sandia)		*0.44*		

On the other hand, the simulations using FGM tables based on Som mechanism show a different behaviour as shown in Table 3. The HR based tables without inclusion of the $\widetilde{Z''^2}$ do ignite whereas the one with $\widetilde{Z''^2}$ fails. All the simulations using ICDF based FGM tables have not achieved ignition except the one with MPI atomization model, which ignites considerably late. The reason for this behaviour is not clear yet. However, some investigations are discussed here.
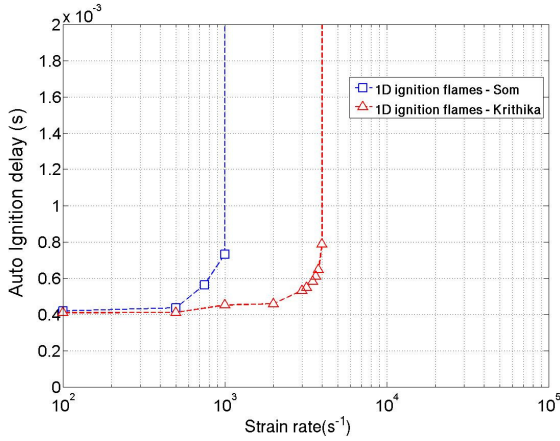
Figure 6: Strain rate effect on ignition, laminar flames at T_{ox} = 900 K, T_{fuel} = 363 K, p = 60 bar.
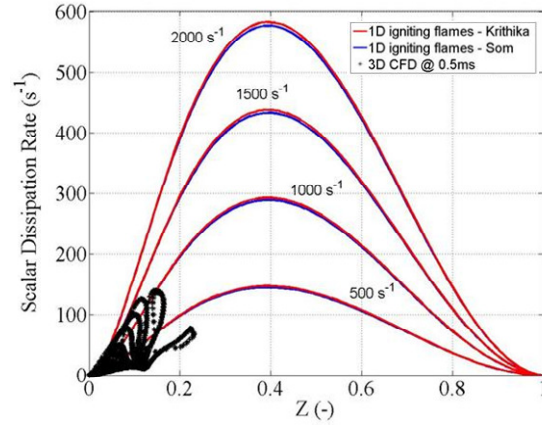

Figure 7: Scalar dissipation rate vs. Z for laminar flames (at different strain rates), and compared with data from 3D CFD.

In case of ICFDs, the ignition behavior is governed by the laminar 1D igniting flames. Figure 6 shows the functional dependency of ignition delay with respect to strain rate for laminar flames, generated using Krithika (red) and Som (blue) mechanism. It is observed that the Som mechanism is highly sensitive with respect to strain rate beyond 1000 s^{-1} whereas Krithika mechanism is able to ignite up to a strain rate of 4000 s^{-1}. The corresponding scalar dissipation rates (χ) for laminar flames are evaluated to compare them with those values from 3D CFD. Figure 7 shows the scalar dissipation rate plot for 1D counterflow flames for strain rates from 500 s^{-1} to 2000 s^{-1}; for Krithika (red) and Som (blue) mechanisms. The figure also shows the cluster of scalar dissipation data points from CFD evaluated at 0.5 ms (typical where ignition starts). As shown in the plot, most of the data points from 3D CFD around Z_{st} are around the region corresponding to a strain rate of 1000 s^{-1} where Som mechanism fails to ignite. Even though the FGM table is generated from a 1D igniting flame at one strain rate (500 s^{-1}), ignition in the 3D CFD situation is not established due to the high level of strain found. The reason why Som mechanism is more sensitive to strain than Krithika mechanism is not clear yet and will be subject to further investigation.

The lift-off length (LOL) is another characteristic of importance for engine combustion. Its definition is still in contemplation in the ECN group. In this work, LOL is defined as the shortest distance measure from the tip of injector to the location in the computational domain where the OH mass fraction reaches to a threshold value of 0.00025. The LOL results are obtained from the simulations that are with the FGM tables based on Krithika, which are indeed igniting.
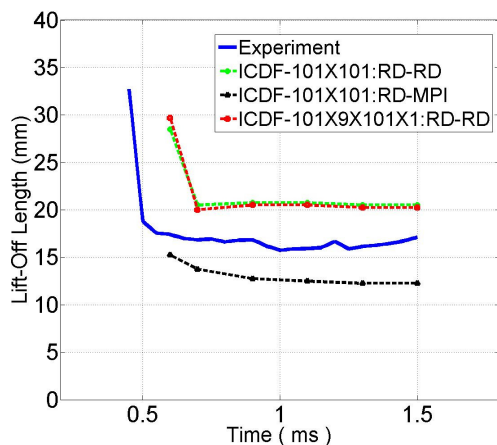

Figure 8: LOL evolutions in time from simulation using ICDFs, and validation with experimental data.
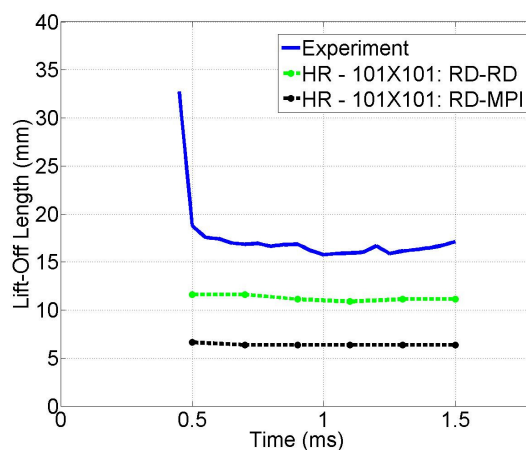
Figure 9: LOL evolutions in time from simulation using HRs, and validation with experimental data.

Figure 8 shows the LOL as a function of time, from the time of ignition to the end of injection (i.e. 1.5 ms), for three different tables, with ICDF tabulation approaches and compared with experimental data. Figure 9 shows the same set of plots for the HR tabulation approach except for the plot for the table with $\widetilde{Z''^2}$, since the

OH threshold (0.00025) value is never achieved. It is evident from the results that LOL in HR based simulations is much shorter than that in ICDF based simulations, which follows the similar trend of ignition delay. It has been also observed in earlier work [14] that LOL is almost a linear function of the ignition delay. The reasons were explained as that high production of y close to nozzle exit due to early ignition in case of HRs. In both methods, atomization model (spray sub-model) influences LOL results remarkably. The LOL is smaller with the *MPI* model when compared to that with the *RD* model. This might be due to the atomization of liquid droplets, which is higher close to injector in case of the *MPI* model while keeping the penetration length comparable with the *RD* model. However, when compared with experimental results, LOL with *RD* is over-predicted and with *MPI* is under-predicted in case of ICDFs. Whereas both atomization models are under-predicted LOL in case of HRs. The effect of $\widetilde{Z''^2}$ on LOL is minor in the ICDF approach.
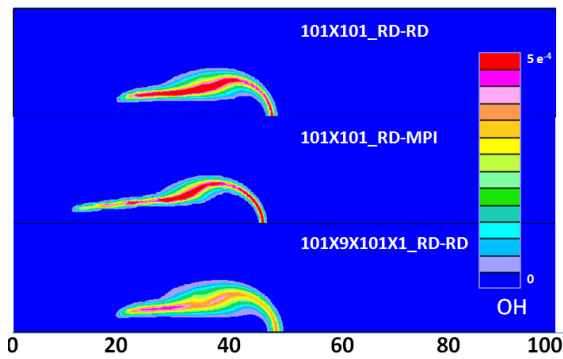
Figure 10: Contours of OH mass fractions at 1.5 ms from simulations using FGM tables by ICDFs.
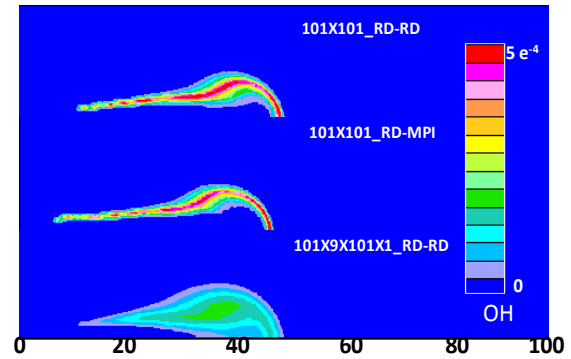
Figure 11: Contours of OH mass fractions at 1.5 ms from simulations using FGM tables by HRs.

Figure 10 and Figure11 show OH contours at 1.5 ms for ICDFs and HRs tabulation approaches respectively. From the contours of OH for tables with and without $\widetilde{Z''^2}$, it is observed that the OH concentrations are lower in case of tables with $\widetilde{Z''^2}$, although the distribution is quite similar due to which no significant effect on LOL is seen. The OH contour of $\widetilde{Z''^2}$ for HRs is significantly different than that for ICDFs, this might be due to the fact that the predicted maximum temperatures from HRs are low compared to that from ICDFs.

Summary and conclusions

Spray A simulations with RANS have been performed. For that reason, various available spray sub-models in STAR-CD have been evaluated. The MPI model has been chosen in addition to Reitz-Diwakar (as atomization model) based on better vapor and liquid penetration predictions. The reacting flow simulations are performed using FGM tables that are generated using the Krithika, and Som mechanisms. Two tabulation approaches i.e. ICDFs, HRs are used and the tables with and without $\widetilde{Z''^2}$ are considered to evaluate the effect of variances. All simulations with Krithika mechanism are igniting whereas some of the cases with Som mechanism fail to ignite. The high sensitivity of ignition to strain rates of this particular mechanism could be the reason; however more investigation is necessary to explain why Som mechanism is more sensitive to strain than Krithika mechanism. The predicted ignition delay with HRs is smaller compared with ICDFs. When compared with experiments, HR tables are under-predictive and ICDF tables are slightly over-predictive. Moreover, LOL predictions follow this trend as well. HR based simulations result in smaller LOL than those with ICDF based simulations, and also under-predicts when compared to experimental values. The LOL from ICDFs with the Reitz-Diwakar model is over predicting compared to experimental values. MPI atomization model shows no effect on ignition delay. However, it is significantly reducing the LOL values in both methods. Hence, it can be concluded that the spray model with Reitz-Diwakar atomization is preferable for its better vapor/liquid penetration and LOL predictions. There is no major effect due to inclusion of $\widetilde{Z''^2}$ in tables on ignition delay, LOL predictions however differences in the OH magnitudes levels observed.

In future work, to evaluate the method and mechanism abilities, it is important to study the sensitivity with respect to change in conditions such as ambient O_2 concentration and temperature.

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