Modeling of Non-Premixed Turbulent Flame Dynamics Using an Open-Source CFD code

Sayop Kim[1,2] and Je Ir Ryu[2,3]

[1]Department of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA, USA
[2]New York University Abu Dhabi, Abu Dhabi, UAE
[3]New York University, Brooklyn, NY, 11201, USA

1 Introduction

A classical textbook description of non-premixed diffusion flame is limited to the analogous problems of equilibrium candle flame. Practically observable flame dynamics in many practical combustors characterizes the intrinsic complexity and non-linear physics paired with the non-equilibrium nature. Ignition and flame stabilization of the non-premixed combustion can be better described from two different perspectives, e.g., turbulent mixing and finite-rate chemistry. Such a multi-physics nature was conceptually sketched in the application of diesel spray flame by Dec [1]. The present study further shed light on the role of local turbulent mixing intensity in the ignition and transient flame structure. To accommodate the turbulent chemistry interaction (TCI) phenomenon in the non-premixed combustion problem, a laminar flamelet concept [2] was employed and extended to modeling a practical diesel-like spray combustion problem. In this study, unsteady flamelet model was implemented into an open-source CFD code, OpenFOAM and verified against the relevant experiment data and further compared with the commercially available CFD solver, CONVERGE. This paper provides insights into general dynamics of the high Reynolds turbulent spray flame using the flamelet model-based TCI model in comparison with a laminar chemistry-based combustion model.

2 Mathematical Descriptions: kinetics-controlled vs. mixing-controlled

Highly non-linear and multi-scale nature of the high Reynolds number turbulent spray flame gives very limited allowance to deterministic analysis, hence reduced order descriptions are demanded in the mathematical modeling platform. Of many bottleneck problems in the modeling descriptions of the turbulent spray flame physics, the finite rate chemistry is a predominant factor. In many practical simulations, the Arrhenius formula-based source term modeling is popular approach to describe the finite rate chemistry without the explicit modeling of sub-grid turbulence closure. This refers to as well-stirred reactor (WSR) model with infinitely fast mixing assumption, hence kinetics control. In general, the WSR model is incorporated within CFD time integration loop to evaluate the turbulent mean reaction rate $\overline{\dot{\omega}}_k = f_k(\overline{Y}_i, \overline{T})$ in species transport equations. Therefore, underlying assumption of this model is to apply homogeneous mixture assumption in grid scale level before chemistry comes into play.

Correspondence to: sayop.kim@nyu.edu

Another source of the modeling errors may arise in the turbulence-chemistry interaction (TCI) aspect, which is notoriously known as highly non-linear and multi-scale physics. To this end, a concept of flamelet model can be used to describe the turbulence scalar flux across the local laminar flame reaction zone where chemically fast reaction takes place, thereby the flame dynamics is mixing-controlled phenomenon. The flamelet model leverages a separation of the chemistry computation from the CFD solution to reduce the computational cost associated with the sub-grid level time and length scale of the local stretched flame. The basic principle of the flamelet model is to view a turbulent diffusion flame as an ensemble of locally unstretched laminar diffusion flamelets. This is valid when the reaction proceeds extremely fast over the mixing residence time within the asymptotically thin layer. Combustion takes place in such a thin layer in the vicinity of an iso-surface of stoichiometric mixture (z_{st}) with the locally high gradient of mixture fraction across the thin reaction zone. Thereby, a reduced-order manifold can be constructed for each of reactive scalars, e.g., Y_k, in a mixture fraction z-space as expressed in Eq. (1) as referred to as flamelet equations:

$$\rho \frac{\partial Y_k}{\partial t} = \dot{\omega}_k + \frac{1}{2}\rho D \chi \frac{\partial^2 Y_k}{\partial z^2}$$

Here, the scalar dissipation rate, χ, appears in the equation and represents the local turbulent mixing intensity. In a counter-flow diffusion flame configuration, for instance, the scalar dissipation rate is indicative of flame stretched rate and plays an essential role in determining the eigenvalue for unsteady flame quenching and auto-ignition, while lacking in the WSR model.

The representative interactive flamelets (RIF) model [3, 4] is an extended version of the flamelet model that executes the flamelet solver (hereafter RIF solver) dynamically and allows the flamelet solution to be incorporated with the CFD solutions. The RIF model utilizes a dynamically computed flamelet library and turbulent mean scalars are calculated by weighing the multiple laminar flamelet solutions with a presumed probability density function (PDF). It is important to note that the RIF model can incorporate the unsteady history of flamelets that would otherwise be unable to follow the rapid change of mixing field, especially in the high-Reynolds number turbulent spray flame.

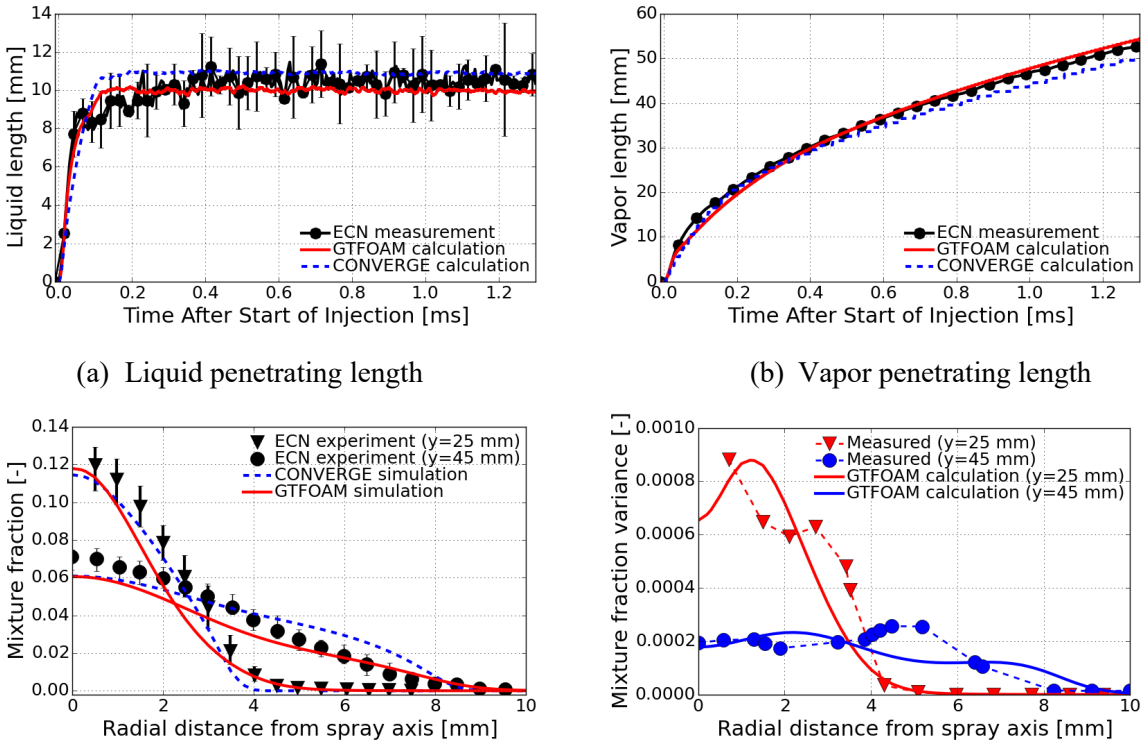
3 Model Implementation into OpenFOAM: GTFOAM

In this study, an independent C++ RIF solver was developed and incorporated in the authors' in-house GTFOAM (Generic Thermal-Fluid OpenFOAM library; available online [5] and technical support provided upon request). The performance of the GTFOAM library was then compared with the results from the CONVERGE CFD solver. Indeed, the original flamelet model concept [3, 4] is to provide the entire reactive scalar solutions including temperature. However, in the RIF solver in the CONVERGE code, the temperature equation in the flamelet reaction space is not directly solved. Instead, the turbulent mean temperature, $\tilde{T}$, in physical CFD space is evaluated once all turbulent mean reactive scalars, $\tilde{Y}_k$, are determined based on the total enthalpy calculation. On the other hand, the GTFOAM follows the original approach in the temperature calculation. The RIF solver executes enthalpy conservation, providing reaction space solutions for respective reactive scalars and enthalpy in the reaction space. In turn, sensible enthalpy in physical space, $\tilde{h}_s(x_i, t)$, is directly calculated by the PDF integration method to provide $\tilde{T}$.

In the spray solver of GTFOAM, major modification was contributed to fix the original OpenFOAM source code inherited errors when calculating the interphase coupling between liquid and gas. The errors may arise due to lacking time scale corrections in the original OpenFOAM spray solver. To reflect the adequate time scale in the source term integration, relevant relaxation time scale [6] was respectively determined for mass, momentum, and energy transfer between gas and liquid phase. The liquid phase physics was modeled in the Eulerian-Lagrangian (E-L) coordinate space; hence the spray was modeled by using the discrete droplet model (DDM) approach.

4 Results and Discussions

Three-dimensional RANS (Reynolds-Averaged Navier-Stokes) simulations were conducted under the ECN Spray-A [7] condition using CONVERGE and GTFOAM as consistent model setup as permitted. The Spray-A condition replicates the high-pressure spray injection under diesel-engine relevant conditions. The *n*-dodecane spray was injected into a quiescent ambient gas within a cubic-volume test chamber (10 x 10 x 10 cm^3) and freely evolves in the chamber; hence free-spray test.



(a) Liquid penetrating length

(b) Vapor penetrating length

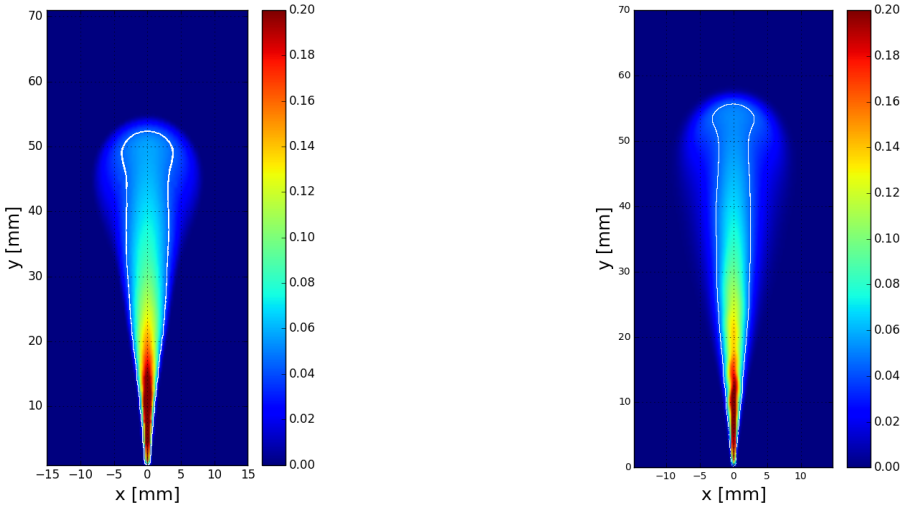
(c) Radial mixture fraction distribution

(d) Radial mixture fraction variance

Figure 1: Non-reacting simulations: spray solver validation against ECN experiment in terms of liquid penetrating length and mixture formation: CONVERGE vs. GTFOAM vs. ECN experiment [7] under non-reacting condition.

Non-reacting Spray-A condition was permitted by inflammable inert gas mixture of N_2, CO_2 and H_2O at 900 K and 60 bar. A close agreement between simulation and experiment during the initial ramp-up period of liquid and vapor penetrations in Figure 1 (a, b) demonstrates that the GTFOAM adequately resolves the mass and momentum exchange between liquid and gas by the time scale correction technique. Figure 1 (c) also shows that the mixture fraction distribution in transverse direction lies within the range of experimental uncertainty for both CFD codes. Figure 1 (d) presents an important indication of the turbulent fluctuating quantities (i.e., mixing intensity) calculated from the GTFOAM simulation only. Figure 2 depicts calculated mixture fraction contour formed by quasi-steady injection and compares the model prediction between two different CFD solvers. As quantified above in Figure 1 (b), the GTFOAM simulation exhibits more elongated vapor length than that of CONVERGE solver. Despite such a difference, overall accuracy of the spray solver predictions is acceptable.

Extended analysis was conducted under the reacting ECN Spray-A condition with initial in-cylinder air composition of O2, N_2, CO_2 and H_2O at 15%, 75.15%, 6.23% and 3.62% respectively by volume at 900 K and 60 bar. This analysis provides several important indications of approximated turbulent mean



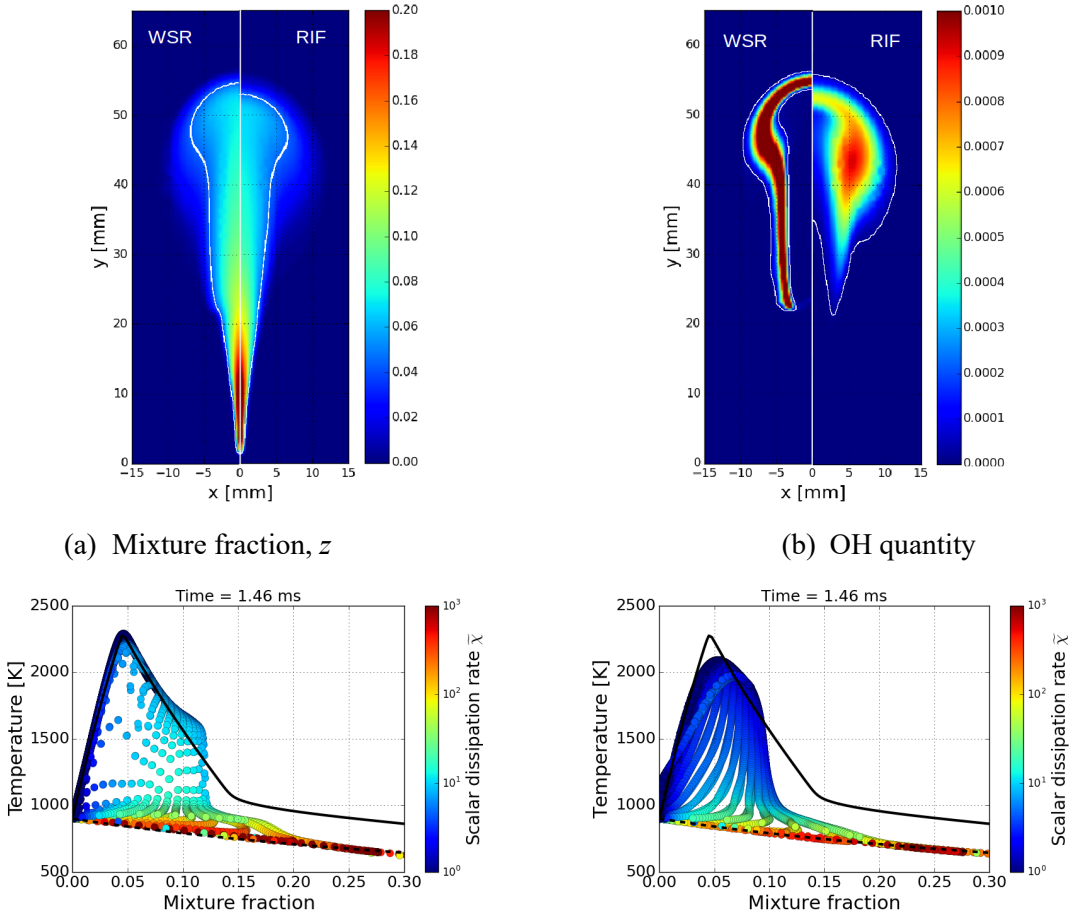
(a) CONVERGE simulation (b) GTFOAM simulation

Figure 2: Non-reacting simulations: contours of mixture fraction calculated by two CFD solvers at 1.46 ms after start of injection. White solid line indicates the stoichiometric mixture formation.

scalar fields in the TCI modeling aspect. One of the key aspects of turbulent combustion dynamics lies in the flame intermittency characteristics. In practical turbulent flows, this is often encountered with unsteady nature of flapping flame brush, which in turn exhibits substantially distributed transverse profile across the spray flame periphery when ensemble averaged (e.g., RANS simulation). In real physics, a scalar measurement across the average spray periphery would yield an intermittent signal due to such a flame flapping motion. Furthermore, there will be a likelihood of finding adiabatic flame temperature over a wide spatial region for the same reason. In this regard, the main conceptual difference between the WSR model and the TCI model (e.g., RIF model in this test) lies in the capability of capturing the intermittency nature. Within the RANS framework, the laminar chemistry WSR model will only show a definitive and instantaneous layer of stoichiometric adiabatic flame zone because of lacking intermittency aspect in the model formulation. Therefore, the key principle of the TCI modeling is to approximate the turbulent "mean" flame profile rather than capturing instantaneous laminar profile in the RANS framework.

Figure 3 (a, b) illustrates the quasi-steady lifted flame captured at 1.46 ms after start of injection. CONVERGE simulations are only presented here to solely brings the aspect of TCI modeling description. One can see different OH profiles across the spray flame periphery, whereas the mixture fraction field appears to be qualitatively similar. It is important to note that the RANS resolved OH mean fraction field with the RIF model reveals substantially wide profile of numerical solution, whereas the WSR model estimates non-zero level of the reaction scalars in the vicinity of stoichiometric mixture with a much narrower span. Also, the approximated OH field with the RIF model shows lower peak of OH level across the stoichiometric line. This provides an indication that the introduction of PDF in the RIF model gives rise to a broader mean reacting scalar profile in the physical space, and consequently a more dissipative solution. Such a rather distributed flame profile by the RIF model supports the idea of intermittency captured by the TCI modeling, because highly unsteady turbulent feature of spray flame may intermittently sweep over a broad range of physical space such that its ensemble-averaged quantity no longer exhibits sharp change in the reaction zone.

Figure 3 (c, d) shows instantaneous flame structure in terms of mixture temperature with respect to mixture fraction z. The stoichiometric mixture is formed at $z = 0.04509$ of n-dodecane fuel under the current test condition. The upper black solid line in the figures follows the variation of equilibrium



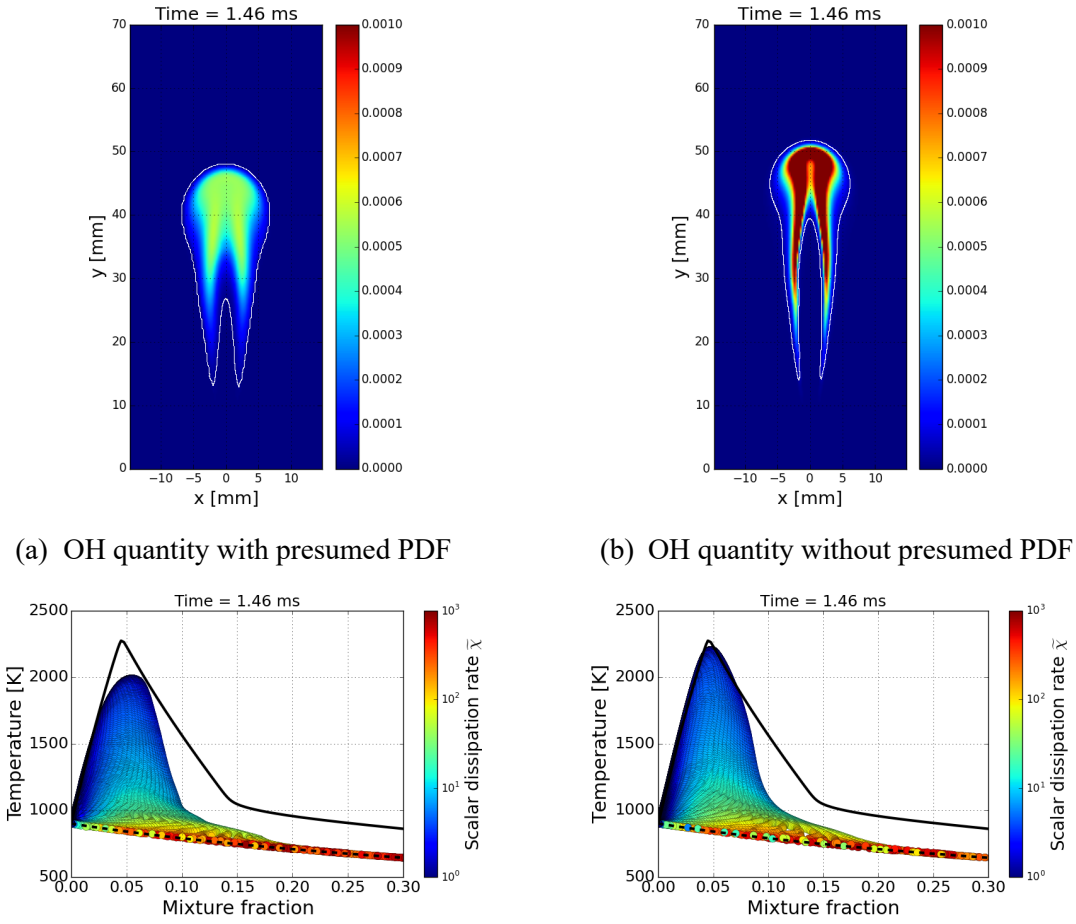
(a) Mixture fraction, z (b) OH quantity

(c) Flame structure by WSR model (d) Flame structure by RIF model

Figure 3: CONVERGE simulations: (a, b) quasi steady turbulent spray flame and (c, d) flame structure with respect to mixture fraction. White solid line in z contour: iso-stoichiometric mixture, White solid line in OH contour: OH level at 2% of maximum steady-state concentration.

temperature (i.e., adiabatic flame temperature) as a function of mixture fraction. The equilibrium temperature was obtained from the zero-dimensional (path-independent) adiabatic, constant volume batch reactor solutions by using the CANTERA solver. The lower black dashed line represents the pure-mixing solution. Thus, individual points in the scatter plots may represent instantaneous progress variable with respect to the equilibrium state. It should be noted that the plots identify overly heated mixture beyond the equilibrium level. This reflects the feature of path-dependent mixing and chemical reaction processes of spray flame in physical space, whereas the batch reactor assumption only considers the mixture fraction variable space.

A noticeable difference found in the flame structures between WSR model and RIF model is obvious by finding some intermediate temperature level between pure-mixing and equilibrium. Points in Figure 3 (c) tend to sit alongside or in the vicinity of mixing line (dashed) and equilibrium line (solid), while Figure 3 (d) identifies significant density of intermediate temperature level. Such a tendency in the WSR model case is attributed to the nature of fast chemistry with no finite rate of mixing. As such, once a mixture element starts to chemically react, it may promptly jump to equilibrium level due to the fast chemistry. However, for the RIF model, the use of presumed PDF integration may generate diffusive solution points as shown in Figure 3 (d). Another difference between two models is found by the stoichiometric mixture temperature. The WSR model predicts definitive adiabatic equilibrium flame



(a) OH quantity with presumed PDF

(b) OH quantity without presumed PDF

(c) Flame structure with presumed PDF

(d) Flame structure without presumed PDF

Figure 4: GTFOAM simulations with effect of presumed β-PDF integration.

temperature around 2,300 K in Figure 3 (c), thus this is evidence of no turbulent scalar mixing in the reaction zone. On the other hand, the RIF model produces lowered peak temperature at this stoichiometric condition since the model combines the effect of local dissipation rate and turbulent intermittency reproduced by the PDF integration method.

To further investigate the effect of presumed PDF integration on predicted flame structure, GTFOAM solver was utilized as it offers a capability of switching PDF integration option by the virtue of its open-source platform, while it is not permitted for the CONVERGE solver. Figure 4 (a ,b) shows calculated flame brush in terms of OH concentration as an indication of high-temperature reaction zone with an option of β-PDF integration turned on and off. Thus, the latter case yields mean flame brush produced by bypassing moment of the PDF integration when estimating mean reactive scalars. One can notice that bypassed PDF integration method in Figure 4 (b) estimated very high concentration and stiff gradient of OH quantity across the spray flame. Therefore, it can be stated that the PDF integration plays an essential role in generating turbulent "mean" flame brush in the ensemble averaged solution. In addition, given the notion that the higher OH concentration indicates more heat release, the case with bypassed PDF integration results in more intense thermal expansion leading to extended flame length along the spray axis.

Figure 4 (c, d) also displays calculated flame structures by setup of GTFOAM solver and the RIF model with and without the PDF integration. The comparison between these two scatter plots exhibits an

outcome of PDF integration in estimating turbulent mean scalars. The presumed PDF method results in lowering peak temperature by 200 K approximately. In addition, one can find that the peak temperature is still below the adiabatic equilibrium flame temperature at stoichiometric condition. This implies that the use of RIF model still applies impact of scalar dissipation rate on the flame structure.

5 Conclusions

In this study, two categories of TCI modeling approach, i.e., kinetics-controlled, and mixing-controlled combustion models (WSR vs RIF) are examined with commercially available CFD code, CONVERGE, and in-house OpenFOAM library, GTFOAM. The results identify major difference between two different combustion models in analysis of the turbulent spray flame dynamics. Major impact was found in the resolved turbulent mean flame brush. The WSR model excludes the effect of higher-order moment terms (i.e., TCI impact) in the reaction source terms, hence the model prediction follows the trend of laminar chemistry dominating flame dynamics. However, the RIF model, based on the flamelet approach, was found to better perform with aid of dynamically resolved flamelet solutions. The RIF model can reproduce the effects of locally stretched diffusion flames. In addition, incorporation of the presumed PDF method enables to provide better resolved characteristics of turbulent flame intermittency, thus the predictions show a wider reaction zone in the RANS simulation, indicating ensemble-averaged flame flapping motions. Finally, the in-house CFD library, GTFOAM solver, incorporates improved time scale solution for the spray solver, hence the code can provide acceptable results of spray dynamics. The GTFOAM solver includes the RIF model test platform with a capability of presumed PDF integration to better account for the turbulent intermittent flame dynamics.

6 Acknowledgement

Authors acknowledge that this study was developed as a part of the dissertation work during the corresponding author, Dr. Sayop Kim's time at Georgia Tech. The development of the GTFOAM library was neither financially supported nor promoted by any grant agencies, therefore free distribution of the source code is highly encouraged upon request via the author's personal email: kim.sayop@gmail.com. Further academic advisory support on the scientific analysis and discussions was provided by Dr. Je Ir Ryu and travel support is granted from the research fund raised by New York University Abu Dhabi.

7 References

[1] J. E. Dec, "A Conceptual Model of DI Diesel Combustion Based On Laser-Sheet Imaging," in *SAE Paper 9708713*, 1997.

[2] F. N. Williams, "Recent Advances in Theoretical Descriptions of Turbulent Diffusion Flames," *Turbulent Mixing in Nonreactive and Reactive Flows,* pp. 189-208, 1975.

[3] H. Pitsch, Y. P. Wan and N. Peters, "Numerical Investigation of Soot Formation and Oxidation under Diesel Engine Conditions," in *SAE Paper 952357*, 1995.

[4] H. Pitsch, H. Barths and N. Peters, "Three-Dimensional Modeling of Nox and Soot Formation in DI-Diesel Engines Using Detailed Chemistry Based On the Interactive Flamelet Approach," in *SAE Paper 962057*, 1996.

[5] S. Kim, "OpenFOAM library for Generic Thermal-Fluid Applications," [Online]. Available: https://github.com/sayop/gtfoam.

[6] C. Kralj, "Numerical Simulation of Diesel Spray Processes," PhD thesis, Imperial College, 1995.

[7] "Engine Combustion Network Experimental Data Archive," [Online]. Available: http://www.sandia.gov/ECN.