Advances in the Application of
Flamelet Generated Manifold for
Diesel Engine Combustion Modeling

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Summary

Advances in the Application of Flamelet Generated Manifold for Diesel Engine Combustion Modeling

The need for robust and predictive numerical diesel combustion models is rising as their contribution in engine research is increasing continuously. The numerical models have higher flexibility for extensive parametric studies and provide 3-dimensional visualizations when compared to advanced experiments, which can significantly reduce the cost and time for proto-type engine development and analysis. However, the modeling of diesel spray combustion and emissions poses various challenges. In the thesis, this problem is segmented into three major components auto-ignition delay, cycle simulations, and emission predictions (mainly soot). The purpose and scope of the thesis is described in Chapter 1. Flamelet Generated Manifold (FGM) is one of the tabulated chemistry approaches, which combines the advantages of the Intrinsic Low Dimensional Manifold method (ILDM) and the flamelet approach. It has been applied to model complex turbulent reactive flows in diesel engines. Spray sub-models in STAR-CD are used to model liquid fuel spray (& vapor) formation, and to that, the FGM tables are coupled using user-defined functions. The FGM tables are generated using Igniting Counter flow Diffusion Flames (ICDF) database or using Homogeneous reactor (HR) database. The chemistry is parameterized as a function of mixture fraction and progress variable, and the effect of mixture fraction variances are accounted by PDF integration. The mathematical description of the approach is presented in Chapter 2.

Firstly, FGM is studied to enhance its capabilities to model igniting diesel spray characteristics. This is done in the context of the collaboration within the Engine Combustion Network (ECN). In Chapter 3, FGM is applied to model single, igniting sprays in a well-conditioned constant volume cell for two different diesel surrogate fuels, namely n-heptane and n-dodecane, and for various ambient conditions. The model predictions with an optimized table resolution build the confidence on the method by showing a good match with experimental data available in the ECN database. The HR based FGM chemistry picks up ignition delay trends where as ICDF based FGM chemistry can predict flame liftoff length trends along with ignition delay predictions. This is due to the fact that ICDF takes account of transport phenomenon. Further, it was also observed that the turbulence closure plays a role in resolving local flame structure more accurately. The model predictions of the ignition delay at lower ambient temperature conditions, however, deviate from the experimental trends due to the higher sensitivity of the chemistry to strain rate.

Subsequently, in Chapter 4. Engine cycle simulations are performed with a moving
mesh in STAR-CD coupled to the tabulated FGM chemistry. The optimum selection of FGM settings, and a validated n-heptane reaction mechanism (more detailed compared to GRI) obtained from Chapter 3 are the key tokens for this work. However, pre-tabulation of the chemistry accounting for the effect of the variable in-cylinder conditions (particularly around ignition) is an imperative and a challenging task. In this work, the FGM is extended with another two lookup variables i.e. pressure and enthalpy to account pressure variations and local heat losses respectively. First, the model with pressure dependent FGM (adiabatic enthalpy level) is applied and the results show that a moderate amount of at least 5 pressure levels (between the pressure at start of injection and peak cylinder pressure) is needed to capture the start of combustion for both conventional and PCCI like combustion modes. In the next step, more enthalpy conditions (obtained from a-priori study) are included at each pressure to represent the effect of local thermal stratification on chemistry. With pressure and enthalpy dependent FGM, considerable improvements are observed with local temperature predictions although the effects on the global parameters like pressure and heat release rate traces are minimal. Further, the model is extended with various levels of \( NO_x \) models in engine cycle simulations and it is found that the pressure and enthalpy dependent FGM model improves \( NO_x \) predictions by capturing the effects due to heat losses.

In the next and final stage, in Chapter 5, a soot model is devised and implemented in this FGM framework. It is a two equation based model, including description of heterogeneous soot formation and oxidation processes. The major question is how well the tabulated-chemistry method can characterize the soot processes. For that reason, first the soot kinetics evaluated with soot \((\phi - T)\) maps before extending it to simulate soot formation in Spray H case. The soot model implemented with current approach reproduces \(\phi - T\) maps (found in literature) and shows encouraging results in capturing the phenomenology of soot formation for Spray H case. However, further validation at various parametric conditions is needed before implementing it to engine cycle simulations since the soot processes are highly sensitive with the change in applied conditions.

Thus, the thesis is focused on advances in the approach to improve the auto ignition predictability, accounting for the in-cylinder conditions during chemistry pre-tabulation for cycle simulations, and emission modeling (mainly soot). The final summary of the advances in the FGM approach is presented in Chapter 6 with conclusions and potential areas to improve for reaching to a model which can be used in industrial engine research, right away.
Chapter 1

Introduction

1.1 Need for active engine research - role of computational models

Power generation using combustion of fossil fuels is a major contributor in meeting the present raising energy needs. According to [Shell-energyscenarios, 2008], as depicted in Figure 1.1 despite of increase in contributions from other energy sources such as nuclear, solar, wind and other renewables, fossil fuel continues its dominant role as a primary source for power generation in coming decades. A large part of this power generation is provided by diesel engines due to reasons like (i) their high power density (ii) low diesel volatility which makes it safe to handle and (iii) since diesel engine is a dependable machine with no ready alternative on the shelf to meet such a wide range of applications, encompassing small scale aircraft engines, automotive, locomotive, marine, gensets and even stand-by power sources for huge data systems which are the heart of today’s industry. However, higher consumption of fuel, global warming and health implications due to the undesirable pollutants emitted from these engines (especially automotive) is a prime concern. In last 3 decades, there have been stringent norms imposed on the engine manufacturers by government regulation agencies which will even get tighter in future. Figure 1.2 shows the European emission standards for heavy duty diesel engines. Therefore, a great need aroused for active and continual engine research. The major potential to improve efficiency and to meet the emission norms is explored by further understanding and optimizing the in-cylinder combustion processes. Since the number of engines introduced every year is huge (17 million of diesel engines only in Europe, which is 24% of entire production in the world [ACEA, 2012]), a great impact can be expected even with small improvements in the engine research and development.

The engine research and development is supported by advanced experiments and computational models. They complement each other, since the advanced experiments are also needed to provide the data in order to validate the computational models which are developed to reduce the need for such experiments for industrial engine development. One advantage of computational models compared to advanced experiments is that computational models can provide more flexibility for extensive parametric studies and for creating complete data with 3-dimensional visualizations which assists proto-type engine analysis. Not only for the development of upcoming engines, but also for the improvement of existing engines like for power up-grades or engine failure analysis i.e. overheating of cylinder
head and liner, computational models can help incomparably. Physical processes can be
decoupled to understand their interaction in order to achieve the better/optimum settings
which might not be possible with experiments alone. Also, with the present scenario of
increasing computational power and fidelity on the model’s performance, the contribution
of computational models in engine research is continuously rising. So, a robust computa-
tion model which can take the account of design variations and predict the parameters of
interest, serves as a directional tool in engine development processes. Hence there will be a
continuous effort to obtain more robust and predictive numerical diesel combustion models.

In this introduction, the diesel engine combustion processes and the types of modeling
approaches are presented briefly. Subsequently current diesel engine combustion modeling
challenges and criteria for a robust and dependable model are discussed. A brief literature
review is then presented to introduce the progress in engine combustion modeling. Finally
the main purpose and scope of the thesis is explained by presenting the outline of the thesis.

1.2 Diesel engine combustion processes

The combustion process in a direct injection (DI) diesel engine can be described as follows:
*a (very) highly pressurized liquid diesel fuel is injected into gas at high pressure and tem-
perature towards the end of compression. The fuel spray breaks up, evaporates and mixes
with the surrounding hot gas. After a certain time the mixture will auto-ignite after which
a lifted partially premixed diffusion flame will establish for as long as fuel injection per-
sists. During this combustion event and even in the expansion stroke undesired components
will be formed. The key processes that are of interest in engine research to improve this
in-cylinder combustion process are fuel spray and mixture formation, combustion (mainly
auto-ignition) and pollutant formation. In the following, these key processes will be defined
in more detail.
1.2.1 Spray and mixture formation

Injection of liquid fuel at pressures approximately 20 times higher than the pressure of the gas (50-100 bar) in the chamber allows it to breakup and atomize into smaller droplets. These atomized droplets evaporate due to surrounding hot gas and then rapidly mix with entrained gas due to the high velocity jet. This entire process is referred to as the spray and mixture formation which is primarily governed by the injector configuration, combustion chamber conditions, volatility of the fuel, etc. The utilization of fresh gas and achieving desired mixing rates can be vital as it establishes the primary requirement for the subsequent combustion event. The better the control is over the formation enabled by the fuel spray, the more efficient the combustion can be. Hence one of the goals of engine research is to characterize these complex and multi-physical spray and mixture formation processes. Spray formation and mixture formation are to a great extent understood at least qualitatively and described comprehensively in e.g. [Heywood, 1988], [Ramos, 1989], [Stiesch, 2003] and [Baumgarten, 2006].

1.2.2 Auto-ignition and combustion

The auto-ignition of the fuel gas mixture occurs as it reaches sufficiently high temperatures. The time taken for the physical (spray and mixing) and chemical (ignition reactions) processes to reach this condition is defined as the ignition delay. This process is highly dependent on the injection details, fuel quality and the gas conditions in the chamber. Auto-ignition is a prelude to the further combustion process. In engine research, the course of the combustion event in diesel engines is denoted by three phases: the premixed (rapid) combustion period, the diffusion (or mixing) controlled combustion phase and finally the post combustion event. The three phases are grossly depicted in the heat-release diagram in Figure 1.3.
In the premixed combustion phase, the already prepared mixture during the ignition delay period will burn quickly causing a steep rise in the heat release rate. This process is controlled by the chemical reaction of the fuel. Subsequently, the mixture prepared further due to the remaining period of the fuel injection event continues burning. Since this burning process is in fact a lifted diffusion flame, mainly controlled by mixing and diffusion, it is referred to as the mixing controlled (or diffusion) combustion. The relevance of the premixed and diffusion phase depends on the load and combustion mode that is applied. Diffusion combustion is dominant in conventional diesel combustion (CDC) mode, which happens at combinations of temperatures and loads where the ignition delay is (much) shorter than the injection duration. The premixed phase, however, is dominant and sometimes the only phase in what is known as Low Temperature Combustion (LTC). This is found in Premixed Charge Compression Ignition (PCCI) or Homogeneous Charge Compression Ignition (HCCI) like combustion modes, characterized by long(er) ignition delays. The time of injection (SOI), the Exhaust Gas Recirculation (EGR) conditions and the reactivity of the fuel determine these modes. Finally, in the late combustion phase, the expansion of the gas slows down the chemical kinetics as the cylinder gas temperature drops. The non-uniform gas composition, consisting of dissociation products at this stage results in the engine-out pollutants. Although phenomenological understanding of the individual processes are gained in literature, the different interactions between the sub processes in the different combustion modes (CDC, LTC) are not well known.

1.2.3 Pollutant formation

The non-ideal condition of mixture composition, temperature and turbulence in diesel combustion results in undesired species such as $CO$, $HC$, $NO_x$, and Soot (Particulate Matter) in the exhaust gas. Due to engine-out levels and their impact on human health and the environment, of major concern are the $NO_x$ and Soot emissions. $NO_x$ comprises of nitric oxide ($NO$) and nitrogen dioxide ($NO_2$). $NO_x$ is majorly formed at high temperatures with
sufficient levels of oxygen. These conditions typically occur in the diffusion flame or in the premixed flame with stoichiometric to lean mixtures (higher oxygen availability). The \( NO_x \) formation mechanism is fairly well understood due to the work by [Zeldovich, 1946]. Soot is defined as the carbonaceous particulates formed during the gas phase combustion at rich mixtures and moderately high temperatures. Soot is the major constituent (along with PAH) of the particulate matter emission in the diesel engine (around 95\%) and the rest is inorganic components. Soot particle formation, growth and the oxidation processes are complex and heterogeneous. Gaining complete understanding of Soot formation and oxidation processes are continuing to be a great challenge and interest to the current research community.

1.3 Modeling aspects of diesel engine combustion processes

The numerical models used to simulate the diesel combustion processes can be classified into three types based on their complexity and required computational cost, as described in [Stiesch, 2003], [Lakshminarayanan and Aghav, 2010]. The first type are the thermodynamics based models, which are highly cost effective as they consider a single lumped amount of mass in the combustion chamber with (in general) very simplified chemical kinetics. Hence it cannot provide any insights into the sub-processes like spray, chemical kinetics, and pollutant formation etc. The second type are the phenomenological models that consider the combustion chamber into multiple zones (at least two) with predefined temperature and equivalence ratio conditions with a certain spatial distribution, and phenomenological description of sub-processes. These models can provide relatively more details including emissions as a function of engine parameters such as EGR, SOI, Compression ratios etc. However their use is limited as they fail to capture the interaction of sub processes and the influence of flow turbulence due to the change in engine geometrical features etc. The third type are the multidimensional model or Computational Fluid Dynamic (CFD) models, which solve the governing equations for conservation of mass, momentum and energy on a computational mesh of the geometry. Detailed sub-models are included for turbulence, spray dynamics, and chemistry. Since these models capture a great level of detail in the spatial and temporal domain, they are time consuming and computationally expensive. On the other hand, these CFD models, with continuously improved predictive quality, are becoming powerful tools in current engine research and development, which aims at a detailed understanding of the sub-processes and interactions. Also with the increase in the present availability of computation power, the development of CFD for diesel engine combustion gained momentum. Still it is important to reduce the computational cost yet keeping the details of sub processes in order to make the usage of modeling in current engine development viable.

Simulations of diesel engine combustion processes will have to account for the inherent sub processes such as turbulent flow, spray formation, combustion and pollutant formation in a dynamically moving computational mesh. The Direct Numerical Simulation (DNS), which is not actually modeling but solving each and every detail, is computationally prohibitive for most practical applications like the diesel engine. The other possibilities are Large Eddy Simulations (LES), where only the filtered scales are modeled, and Reynolds Averaged Navier Stokes (RANS) where the averaged quantities are solved [Sadiki et al., 2006]. Both are significantly less expensive than the DNS approach. Unless the interest
is to look into the cylinder to cylinder or cycle to cycle unsteady flow variations, RANS simulations can provide adequate details for diesel engine combustion. Hence current industrial engine development is highly favored towards RANS based approaches. In the spray formation models, the injection of the liquid fuel (disperse phase), its break up and atomization, droplet movement, collision, interaction with the wall and evaporation have to be modeled in a turbulent continuous phase flow. This multiphase flow interaction has to be incorporated. The existing CFD spray sub models, which are based on a well-understood phenomenology of the spray dynamics, can predict the mixing field satisfactorily [Reitz, 1987, Kong et al., 1999]. However, it must be noted that in most implementations in commercial codes the computational grid size and solver time step play an important role to achieve accurate results.

Figure 1.4: Range of number of species and reactions from existing chemical mechanisms for hydrocarbon fuels [Lu and Law, 2009].

The combustion modeling of diesel like fuels (heavy hydrocarbons ranging from $C_{10}H_{20}$ to $C_{15}H_{28}$) deals with more challenges as it has to account for the large amount of elementary reactions amongst a large number of intermediate species. Figure 1.4 illustrates the range of currently available detailed and skeletal mechanisms for hydrocarbons (upto $C_{16}$) including the years when they were developed [Lu and Law, 2009]. Some of diesel surrogate fuels such as $n$-heptane, $n$-decane, $n$-dodecane, $i$-octane etc., are also included. In addition to computational expense involved in transporting this large set of species in the CFD model, the wide span of their chemical time scales makes it computationally stiff. Figure 1.5 shows the range of the time scales for turbulent flows and the chemistry involved in diesel combustion. Apart from these numerical parameters, modeling of turbulent flow interaction with chemistry is also another challenge in combustion modeling since it is also vital to account for the flow field influence on the chemical source terms. Furthermore, the length scales of combustion events are in general smaller than the Kolmogorov length...
scales. This implies in any turbulent modeling approach that the flame structures are not resolved on the mesh scale. Consequently special attention has to be paid to the accurate modeling of the so-called Turbulent Chemistry Interaction (TCI).

![Chemical time scales vs physical time scales](image)

**Figure 1.5:** Timescales involved for various processes in diesel combustion [Energetics, 2008].

The modeling of pollutant formation poses another challenge since their time scale range is different from that of the turbulence and the chemistry associated with fuel conversion. The prerequisite for these models is capturing accurate local temperatures and species distributions and hence the use of detailed chemistry can be desirable. Besides, in case of soot modeling, the formation and oxidation processes are complex and heterogeneous and mostly the phenomenology is not completely understood.

On the other hand, coming to practical applications, the combustion process in recent engine concepts like PCCI can pass into multiple regimes which can be premixed, diffusion or partially premixed or combinations of them during the parametric variation such as time of injection, EGR, temperature and density. Hence the model should be able to account for changes in these combustion regimes, in order to have wider applicability.

In recent literature, a lot of work is carried out in this research field of diesel combustion modeling and with the same focus, the present thesis also attempts to contribute to it.

### 1.4 Diesel engine combustion modeling - Literature review

There are several approaches found in literature for 3D CFD modeling of diesel engine combustion starting from the first ever attempts which are reported in the work of [Cartillieri and Johns, 1983]. With the development of detailed sub models, the recent models can be identified based on their description for the ignition process, flame structure, detailed chem-
ical kinetics and the treatment of the turbulence-chemistry interaction (TCI). The simplified models, with respect to ignition and TCI, like the Shell/Characteristic Time Combustion (CTC) [Halstead et al., 1977, Abraham et al., 1985], Eddy Breakup Model (EBU) [Spalding, 1971], Eddy Dissipation Model (EDM) [Magnussen and Hjertager, 1977] and their variants are developed based on the assumption that the combustion chemistry is governed by the turbulent mixing rate. These models are very efficient due to the severe simplification in chemistry in combination with tunable parameters; however it was shown in [Singh et al., 2006] that they are not applicable in the Low Temperature Combustion (LTC) modes in which the effect of detailed chemistry is dominant and when species or pollutant formation is of prime interest. With further advancements, these models with the same approach but involving detailed chemical kinetics are the so-called well-stirred reactor models can be found in [Kong et al., 2001]. The reduction of chemical mechanisms with maintaining the accuracy to reduce the computation cost, and also accounting turbulent-chemistry interaction are additional challenges in this models which are found in [Nordin, 2001, Tao and Chomiak, 2002].

With the conceptualization of the flamelet theory [Peters, 1984], the decoupling of chemical kinetics and turbulence is achieved within the assumption that on a local scale the turbulent flame can be adequately described by a collection of simple laminar flames. The validity of this philosophy is attributed to the fact that chemical time scales are significantly smaller than the turbulent time scales. For steady turbulent flame applications [Pope, 1985, Roekaerts et al., 2006, Haworth, 2010], the Turbulence Chemistry Interaction (TCI) is achieved in various ways, either applying a pre-sumed shape pdf’s or transported pdf’s. Due to its transient nature of diesel combustion, several modifications to the original approach have been proposed and applied. Representative Interactive Flamelet (RIF) [Pitsch et al., 1996, Peters, 2000, Gopalakrishnan and Abraham, 2003] and Transient Interactive Flamelet (TIF) [Lehtiniemi et al., 2008] are examples of these. In these approaches a series of representative time-dependent 1D laminar diffusion flames are computed on the fly adapting to the local conditions. However, determining the optimum number of representative flamelets can be an important feature. The optimum is defined by the tradeoff between the computational cost (number of flamelets) and accuracy of such models. On the other hand, there are flamelet-based models that adopt unsteady flamelet libraries in combination with sensible enthalpy as a progress variable approach [Lehtiniemi et al., 2005]. Building a huge library considering all in-cylinder conditions needs enormous computation time and power. There are also many mathematically advanced models for turbulent closure of diesel combustion modeling which can be found in literature such as transported PDF model [Kung and Haworth, 2008], Conditional Momentum Closure model (CMC) [Wright et al., 2009, Bolla et al., 2014], with considerable computational expense.

In this thesis the Flamelet Generated Manifold (FGM) method is employed. The FGM is one of the flamelet based chemistry tabulation methods to model turbulent reacting flows. This tabulation technique is developed [van Oijen, 2002] based on a theoretical basis similar to that of well known mathematical reduction method Intrinsic Low Dimensional Manifold (ILDM) [Maas and Pope, 1992], which proposes that the detailed chemistry system can be identified by a low dimensional manifold in composition space. However, in ILDM, the definition of the manifold is based on a rigorous chemical timescale analysis in absence of the physical processes i.e. convection and diffusion, which limits the applicability. In FGM, flamelets are used to define the manifold, which is the link with the earlier mentioned
flamelet methods. The parametrization of the manifolds, however, is similar to that employed in the ILDM approach, i.e. with progress variables. In literature, FGM is widely applied for modeling various combustion phenomena [van Oijen and de Goey, 2004, Bongers, 2005], also including unsteady effects and Lewis number effects [Delhaye et al., 2009, Vreman et al., 2009] and proved to be a computationally efficient method. Since FGM allows pre-tabulating the variables of interest based on detailed chemistry, it is an attractive approach to model multivariate processes such as ignition, combustion and pollutant formation in diesel engines. In the recent past, the first implementation of FGM to diesel engine combustion showed promising directions [Bekdemir et al., 2009]. However, the accurate prediction of ignition at wide in-cylinder conditions, incorporating local heat loss effects, and the incorporation of detailed pollutant formation are not yet explored. These aspects are studied and addressed in this thesis work.

1.5 Purpose and scope of this thesis

The main purpose of the thesis is to enhance FGM model capabilities to achieve a robust and complete model to predict diesel engine combustion processes. Diesel engine combustion is complex and rich due to its diverse processes with constant interactions which necessitate a systematic approach to make improvements at each stage of sub-processes modeling. For instance, although the main focus of the research is the modeling of combustion, setting up the optimum model for the fuel-air mixing fed by the liquid spray is a vital prerequisite and developing such models is out of the scope of current work. For this purpose, a dedicated engine CFD code (STAR-CD) is used throughout the entire thesis. Here RANS based turbulent models and special spray models suited for engine simulations are implemented.

Auto-ignition is a key process in the diesel engine combustion as it determines the initiation of the combustion event and the consequent pollutant formation. The FGM method is implemented with tabulated chemistry based on igniting flamelets to account for auto-ignition phenomena. Two different configurations are applied to generate the database and the effect on predictability is studied. Although this approach proved its ability to capture ignition delay principally, the potential enhancements (for instance, table resolution and TCI) in this inherent implementation features need to be explored. It is in order to improve the predictability of the model for the ignition characteristics at a wide range of engine-like conditions. As the chemical structure of the diesel fuel is largely unknown, the fuel is approximated by surrogates, which are simpler representations of the actual fuel at hand. Even more so, in the Engine Combustion Network (ECN) [ECN, 2012] dedicated experiments are performed with some of these surrogates, to reduce modeling uncertainties. The network data for \( n \)-heptane and \( n \)-dodecane are extensively used for the FGM model’s assessment.

The fundamental advantage of FGM in using diesel engine cycle simulations is pre-tabulation of the detailed chemistry which leads to large gains in computational time. However, the question is how to incorporate the effect of heat losses on chemistry in pre-tabulation along with the variable pressure and temperature conditions in an engine with moving piston. Inclusion of additional dimensions (progress variables) to the FGM, the way to find the local state identifier in CFD for lookup, and the optimum number levels needed are the prime interest of this study. This is first time to implement heat loss model in FGM framework for engine cycle simulations. The improvements in the predictions
corresponding to the flame structure, species concentrations and local temperature predictions are examined. For the pollutant formation accurate predictions of these fields are a pre-requisite.

The implementation of these pollutant formation sub-models within the FGM approach is covered in the final stage of the thesis work. With relatively well understood $NO_x$ formation processes and well documented model availability in literature for diesel engine combustion, it is possible to implement $NO_x$ model in FGM. Soot modeling poses a more significant challenge due to its complexity involved with its formation processes and the lack of complete understanding in literature. A soot model which includes more detailed processes is developed and analyzed with respect to the often employed $\phi - T$ maps [Kitamura et al., 2002]. This implementation of soot model in FGM framework is also first time and new. Further, simulation of the soot fields of one of the ECN spray will be performed and the results are compared with available test data.

1.6 Outline

The brief outline of the thesis is given here. The mathematical description of the basic FGM methodology is presented in Chapter 2. The theoretical basis for the FGM implementation is also presented. In Chapter 3, the implementation of FGM to model single, igniting sprays for two different ECN target flames with surrogate diesel fuels being $n$-heptane and $n$-dodecane is presented. An a-priori study to obtain best combination of model settings for non-reacting spray, a study on the effect of tabulation methods and optimization study of FGM table features is presented here also. In the further work with Spray A condition, the FGM model is evaluated for a wide set of conditions. Subsequently, in Chapter 4, engine cycle simulations are performed with a moving mesh (sector) in STAR-CD with optimum selection of FGM settings, and a validated $n$-heptane reaction mechanism obtained from the work presented in Chapter 3. The FGM is extended with another two lookup variables i.e. pressure and enthalpy to account for pressure variations and local heat losses, respectively. First, the pressure dependent FGM model is validated for two different combustion modes i.e. CDC and PCCI case. Then, the pressure and heat loss dependent FGM is applied for CDC case and the improvements in predictions (mainly $NO_x$) are studied and the implications are discussed.

Further, in Chapter 5, a more detailed soot model, which includes heterogeneous soot processes such as nucleation, surface growth, coagulation, and oxidation, is developed. The predictions of the soot model based on two (soot volume fraction, particle number density) equations are compared to so-called $\phi - T$ maps found in literature. To limit the amount of modeling uncertainties in full engine cycle simulations and also due to the availability of detailed experimental data, the model is applied to sprays in a constant volume combustion chamber as discussed in the work of Chapter 3. The simulated soot volume fraction is then validated against the available experimental data from ECN.

The final summary of the enhancements in the FGM approach is presented in Chapter 6 with conclusions and discussing the potential areas to improve.
Chapter 2

Methodology

In this chapter, first the basic system of conservation equations i.e., Navier Stokes equations for reacting flows are described along with combustion chemistry modeling. In subsequent section, the derived averaged form i.e., Reynolds Averaged Navier Stokes (RANS) equations for spray induced turbulent reacting flows are presented. The various sub models for turbulence and spray formation are summarized before describing the combustion modeling. Finally, the methodology of FGM and its implementation to model combustion which is the main focus of the thesis is presented in detail.

2.1 Conservation equations for reacting flows

The application of conservation laws of mass, momentum, energy and species mass fractions for a multi-dimensional reacting flow problem results in a system of partial differential equations. These are widely known as the Navier Stokes equations. In this section, these equations are briefly described.

The mass conservation equation is given by,

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0, \]  

(2.1)

which is also known as the continuity equation, and the Einstein summation convention is used (also throughout the chapter). Here, \( \rho \) is the mass density, \( t \) is the time, \( u_i \) is \( i^{th} \) component of velocity \( u \) and \( x_i \) is a cartesian coordinate with \( i=1,2,3 \).

The momentum conservation equation is given by,

\[ \frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_i} (\rho u_i u_j) = - \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i} (\tau_{ij} - \rho + \rho g) \]  

(2.2)

where \( p \) is the static pressure, \( \tau_{ij} \) is the stress tensor and \( g_i \) is the acceleration due to gravitational force.

The energy conservation equation in terms of static enthalpy yields,

\[ \frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_i} (\rho u_i h) = \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} - \frac{\partial q}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j}, \]  

(2.3)
in which $h$ is the static enthalpy and $q$ is diffusion energy flux. $h$ is also referred to as the chemico-thermal enthalpy and it is defined as follows,

\[
h = \sum_{k=1}^{N_s} Y_k h_k = \sum_{k=1}^{N_s} Y_k \left[ \left( \triangle h^\circ_f \right)_k + \int_{T_r}^{T} c_{p,k}(T')dT' \right]. \tag{2.4}
\]

The first component on the right hand side is the chemical part, where $(\triangle h^\circ_f)_k$ is the formation enthalpy of species $k$ at a reference temperature $T_r$. The second component is the thermal or sensible part, where $c_{p,k}$ is the specific heat of a species $k$ which is a strong function of temperature. The system involves $N_s$ species, and the mass fraction of a species $k$ is denoted as $Y_k$.

In reacting flows, the species are formed and consumed due to the reactions. Hence, each species will hold a conservation equation which can be cast in the following form,

\[
\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) + \frac{\partial}{\partial x_i}(\rho U_{k,i} Y_k) = \dot{\omega}_k, \quad k \in [1, N_s], \tag{2.5}
\]

Based on mass conservation,

\[
\sum_{k=1}^{N_s} Y_k = 1. \tag{2.6}
\]

Here, $\dot{\omega}_k$ is the chemical source term. The description of $\dot{\omega}_k$ is given in the sub-section further-on. $U_{k}$ is known as the diffusion velocity of species $k$. Many formulations are applied for example Fick’s law, Hirschfelder and Curtiss approximations. In general, it is approximated with a Fick-like expression.

The above stated total number of balance equations is not sufficient to solve all unknown quantities. A state equation is used to close the system of equations. Generally, the ideal gas law approximation is applied to combustion problems which reads,

\[
p = \rho R_u T \sum_{k=1}^{N_s} \left( \frac{Y_k}{M_k} \right), \tag{2.7}
\]

where $R_u$ is the universal gas constant, $8.314 \ Jmol^{-1}K^{-1}$, where $M_k$ is molecular mass of species, $k$.

**Chemical kinetics**

The combustion event in chemically reacting flows is defined by the chemical kinetics of the system which consists of $N_s$ species with $N_r$ reactions. The source term of species $k$, $\dot{\omega}_k$ in equation (2.5) is obtained from this chemical system.
A general form to represent the entire chemical reaction system is,

$$\sum_{k=1}^{N_s} \nu'_{k,l} M_k \stackrel{k_{f,l}}{\rightleftharpoons} \sum_{k=1}^{N_r} \nu''_{k,l} M_k, \quad l \in [1, N_r].$$

(2.8)

Here, species $k$ is represented by $M_k$ and, $\nu'_{k,l}$ and $\nu''_{k,l}$ are the stoichiometric coefficients for forward and reverse reactions whose reaction rate coefficients are denoted as $k_{f,l}$ and $k_{r,l}$, respectively.

The reaction rate coefficient for any reaction is defined with the Arrhenius expression:

$$k_l = A_{f,l} T^{\beta_l} \exp\left(-\frac{E_{a,l}}{R_a T}\right) \quad \text{or} \quad A_{f,l} T^{\beta_l} \exp\left(-\frac{T_{a,l}}{T}\right),$$

(2.9)

where $A_{f,l}, \beta_l$ are the pre-exponential rate constants. $E_{a,l}, T_{a,l}$ are known as the activation energy and the activation temperature, respectively.

The reaction rate for the reaction $l$ is defined as,

$$r_l = k_{f,l} \Pi_{k=1}^{N_s} [M_k] \nu'_{k,l} - k_{r,l} \Pi_{k=1}^{N_r} [M_k] \nu''_{k,l},$$

(2.10)

in which $[M_k]$ - molar concentration of the reactant species $k$.

The net source term for species $k$ in general may have contributions from all $N_r$ chemical reactions, hence $\dot{\omega}_k$ becomes

$$\dot{\omega}_k = M_k \sum_{l=1}^{N_r} (\nu''_{k,l} - \nu'_{k,l}) r_l, \quad k \in [1, N_s].$$

(2.11)

The reaction kinetics details (all elementary reactions of the species, rate constants and activation temperature/energy) for the oxidation process of fuel is provided in a so-called reaction mechanism. For practical fuels like diesel, the chemical structure is not completely known due to large number of components which may vary based on its origin of production. So, alternatively, surrogate fuels [Pitz and Mueller, 2011] are proposed with a few heavy hydrocarbons such as $n$-heptane or $n$-dodecane to mimic the ignition and oxidation behavior of real diesel fuel. The chemical mechanism of such surrogate fuels consists of hundreds of species and thousands of reactions (see Figure 1.4). In this thesis, mainly two detailed reaction mechanisms (one for $n$-heptane, and another for $n$-dodecane) are employed for diesel modeling, although a few other mechanisms are used for comparison. For $n$-heptane surrogate fuel, the detailed reaction mechanism of Andrae [Andrae, 2008] consisting of 633 reactions with 137 species is being used. Whereas, for $n$-dodecane surrogate fuel, the detailed mechanism from Narayanaswamy and Pitsch [Narayanaswamy et al., 2013] which consists of 253 species and 1437 reactions is applied.

Numerical simulation of turbulent reacting flows by applying the above set of conservative equations for a practical system like a diesel engine poses mainly two challenges.
Firstly, the computational stiffness of the complex chemical kinetics for diesel surrogate fuels. Typically the chemical reactions involve a wide range of time scales while each species participates in many of such reactions. Hence solving set of equations makes a computationally stiff system. This problem is circumvented by either chemical or mathematical reduction methods. In chemical reduction methods [Peters, 1991, Smith et al., 2012], the reaction mechanism is reduced by removal or replacing of the species and processes which are 'fast' and do not take a significant role in the flow-chemistry interactions. However, a huge a-priori knowledge on the species and reactions is required while the reduced mechanism’s validity is limited to the conditions for which it is generated. In mathematical reduction models such as Intrinsic low dimensional manifolds (ILDM) [Maas and Pope, 1992] and Computational Singular Perturbation (CSP) [Lam and Goussis, 1994], the entire chemistry system is described by a few controlling variables. These variables are based on the assumption that 'fast' species quickly relax to the path of rate controlling species or processes. This path is also known as a low-dimensional manifold. However, the method may not be applicable where the diffusion and convection processes are dominant in chemical kinetics for instance in low temperature chemistry, or extinction or re-ignition processes. Another set of methods is flamelet based methods which are introduced to reduce the computational cost in turbulent reacting flows. It assumes that the reaction layer is very thin and are not disturbed by local flow conditions (e.g. turbulent eddies). Hence a multidimensional flame can be represented by an ensemble of locally 1D flames (so-called flamelets). This approach allows to decouple the computations of the flow from computations of detailed chemistry. The method used in this thesis, Flamelet Generated Manifold (FGM) [van Oijen, 2002], is one of the flamelet based chemistry tabulation methods [Gicquel et al., 2000, Lehtiniemi et al., 2005]. It is different from the classical flamelet methods in the way the tabulation is performed. The detailed description of the FGM and CFD implementation is presented in Section 2.3.

The second challenge is resolving the turbulent flow field in-conjunction with a two-phase flow (caused by the liquid spray) within the in-cylinder combustion chamber. The first and most accurate approach is Direct Numerical Simulations (DNS), in which the chosen computational cell size is fine enough to resolve smallest length scales i.e., Kolmogorov length scales. These length scales decrease with the increase in Reynolds number [Pope, 2000]. The cell size should also fulfill the requirement to resolve the droplet evaporation. Based on these conditions, the desired number of grid cells for a typical real engine combustion chamber is around $10^{12}$ which implies enormous computation resources and makes the DNS simulations prohibitive for engine simulations [Stiesch, 2003]. The second approach is Large Eddy Simulations (LES) where large scale eddies will be resolved and the effect of small eddies will be modeled using sub-grid scale (SGS) models. Compared to a DNS, LES is computationally less expensive while the unsteady flow effects such as cycle to cycle variations in internal combustion engines will be captured. However, the importance of specific selection of sub-grid scale models and higher computational efforts constrains the LES approach mainly to fundamental research tasks. The third and most commonly used approach for engineering applications is the Reynolds Averaging Navier Stokes (RANS) approach where the mean quantities are resolved and the unsteady turbulence effects on these quantities are included by the sub-models. This approach is advantageous due to its applicability for any configuration, with feasible computational efforts. Therefore, many of the codes used by industry are based on RANS. Although the application of Large Eddy Simulations
LES in modeling engine processes is gaining interest but still needs high computational efforts to include multiphysical processes (such as spray, emission formation etc.). Hence, in this thesis only RANS based simulations are used for modeling engine processes. In the next section, the RANS system of equations and the sub models are described in detail.

2.2 RANS for spray induced turbulent reacting flows

The time averaging (over entire turbulent spectrum) is applied to the instantaneous conservation equations (2.1 to 2.3, 2.5) to obtain the RANS system of equations for the mean quantities. This averaging procedure introduces unknown terms which will be modeled using turbulence models and are discussed in Section 2.2.1. In Reynolds averaging, the instantaneous quantity ($\psi$) is split into a mean ($\bar{\psi}$) and a fluctuating ($\psi'$) component so as

$$\psi = \bar{\psi} + \psi'. \tag{2.12}$$

However, this Reynolds decomposition leads to many unclosed terms if it is applied to variable density flows such as reacting flows. Hence, to avoid this, Favre averaging is introduced in which mass-weighted averaging is applied. In Favre decomposition, the instantaneous quantity ($\psi$) = mean quantity ($\tilde{\psi}$) + fluctuating quantity ($\psi''$) where, $\tilde{\psi} = \rho \bar{\psi}$. The presence of a dispersed (liquid) phase in the continuous (gas) phase contributes to mass, momentum and energy conservation equations via additional source/sink terms. The interaction is modeled using the spray sub-models which are explained in Section 2.2.2.

The RANS system of conservation equations for the spray induced turbulent reacting flows read as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \bar{u}_i)}{\partial x_i} = \bar{S}_m, \tag{2.12}$$

$$\frac{\partial \rho \bar{u}_i}{\partial t} + \frac{\partial (\rho \bar{u}_i \bar{u}_j)}{\partial x_i} = - \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho \tau_{ij}}{\partial x_i} - \frac{\partial \rho \bar{u}_i \bar{u}_j}{\partial x_i} + \rho g_i + \tilde{S}_f, \tag{2.13}$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial (\rho \bar{u}_i \bar{h})}{\partial x_i} = \bar{\tilde{u}}_i \frac{\partial \rho}{\partial x_i} - \frac{\partial \rho \bar{u}_i \bar{h}}{\partial x_i} + \rho \tilde{u}_i \bar{h} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \tilde{S}_h, \tag{2.14}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial (\rho \bar{u}_i Y_k)}{\partial x_i} = - \frac{\partial \rho U_k, Y_k}{\partial x_i} + \rho \bar{u}_i \bar{Y}_k + \bar{\tilde{u}_i} \bar{Y}_k + \tilde{\omega}_k + \tilde{S}_k. \tag{2.15}$$

The laminar viscous tensor $\tilde{\tau}_{ij}$ in equation (2.13) is modeled using Stokes’ law for a Newtonian fluid with average quantities

$$\tilde{\tau}_{ij} = -\mu \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \right]. \tag{2.16}$$
The laminar heat conduction flux $q_i$ in equation (2.14) is expressed by Fourier’s law in terms of average quantities,

$$\bar{q}_i = -\lambda \frac{\partial \bar{T}}{\partial x_i} = -\mu \frac{\partial \bar{h}}{Pr_k \partial x_i}. \quad (2.17)$$

The laminar species mass diffusion flux $\rho U_{k,i} Y_k$ in equation (2.15) is calculated using Fick’s law in terms of average quantities,

$$\bar{\rho} U_{k,i} Y_k = -\bar{\rho} \tilde{D}_k \frac{\partial \bar{Y}_k}{\partial x_i}, \quad (2.18)$$

where $D_k$ is the molecular diffusion coefficient of species $k$ and is here simply characterized by the Lewis number (defined as the ratio between thermal and species mass diffusion),

$$D_k = \frac{\lambda}{\rho c_p L e_k} = -\frac{\mu}{S c_k} \frac{\partial \bar{Y}_k}{\partial x_i}. \quad (2.19)$$

In this study, we assume $Le_k = 1$. The terms $t_1, t_2, t_3$ in the equations (2.13 - 2.15) are treated separately in the next section.

### 2.2.1 Turbulence modeling

The terms $t_1, t_2, t_3$ appear due to the averaging process, and are known as the Reynolds stress, turbulent heat conduction flux and turbulent species diffusion flux, respectively. These terms are considered to take account of the effect of turbulence eddies on the mean flow quantities. Since these terms can not be calculated based on the general laws, many approaches are being used in engineering applications. The most widely used approach is the Eddy viscosity approach.

In this, the Boussinesq approximation is applied for the Reynolds stress in analogy with the viscous stress tensor form as shown in equation (2.16). The turbulent heat and species diffusion is modeled using a classical gradient approach analogous to the formation for the laminar heat and species diffusion as shown in equation (2.17), (2.18):

$$\bar{\rho} u_i'' u_j'' = -\mu_t \left[ \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right] + \frac{2}{3} \bar{\rho} k, \quad (2.20)$$

$$\bar{\rho} u_i'' h'' = -\frac{\mu_t}{Pr_t} \frac{\partial \tilde{h}}{\partial x_i}, \quad (2.21)$$

$$\bar{\rho} u_i'' Y_k'' = -\frac{\mu_t}{S c_k t} \frac{\partial \tilde{Y}_k}{\partial x_i}. \quad (2.22)$$
Here, $\mu_t$ is the turbulent dynamic viscosity which is a property of the turbulence flow, $Pr_t$ is the turbulent Prandtl number and $Sc_{kt}$ is the turbulent Schmidt number of species $k$.

The main objective of the eddy viscosity models is to estimate $\mu_t$. Many models with a different degree of complexity have been proposed based on the number of PDEs that have to be solved [Poinsot and Veynante, 2012]. The Prandtl mixing length model (also known as Zero-equation model) and the Prandtl-Kolmogorov model (also known as One-equation model) are the simplest models available. However, in this study the $k-\epsilon$ model (two-equation model) is used due to its robustness and yet relative simplicity. In this approach, the turbulent dynamic viscosity is estimated as,

$$\mu_t = c_\mu \bar{\rho} k^2 / \epsilon, \quad (2.23)$$

where $k$ is turbulent kinetic energy which is defined as $\frac{1}{2} \sum_{i=1}^{3} u_i'' u_i''$. The variants of these models studied in this thesis are the standard (high Re) model, RNG model, and the Realizable model. In principle, they all solve two transport equations for $k$, $\epsilon$ with only a slight different formulation of equations. The equations for the standard $k-\epsilon$ model are presented here and the details of the other $k-\epsilon$ models can be found in [Sta, 2008]:

$$\frac{\partial}{\partial t} (\bar{\rho} k) + \frac{\partial}{\partial x_i} \left[ \bar{\rho} \bar{u}_i k - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] = \mu_t (P + P_B) - \bar{\rho} \epsilon - \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_i} + \rho k \right) \frac{\partial u_i}{\partial x_i}, \quad (2.24)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \epsilon) + \frac{\partial}{\partial x_i} \left[ \bar{\rho} \bar{u}_i \epsilon - \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] = C_{\epsilon 1} \frac{\epsilon}{k} \left[ \mu_t P - \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_i} + \bar{\rho} k \right) \frac{\partial u_i}{\partial x_i} \right]$$

$$- C_{\epsilon 2} \bar{\rho} \frac{\epsilon^2}{k} + C_{\epsilon 3} \frac{\epsilon}{k} \mu_t P_B + C_{\epsilon 4} \bar{\rho} \epsilon \frac{\partial u_i}{\partial x_i}, \quad (2.25)$$

where the $\sigma_k$, $\sigma_\epsilon$ are the turbulent Prandtl number for $k$ and $\epsilon$ respectively, while $C_{\epsilon 1}, C_{\epsilon 2}, C_{\epsilon 3}$ and $C_{\epsilon 4}$ are model coefficients. The default values of these constants are given in table 2.1.

The first terms on the righthand side of the equation (2.24) refers to the production term due to shear stresses and buoyancy forces. Here,

$$P \equiv \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j},$$

$$P_B \equiv - \frac{g_i}{\sigma_{h,t}} \frac{1}{\rho} \frac{\partial u_i}{\partial x_j}.$$

The second and third terms refer to viscous dissipation, amplification or attenuation due to
Table 2.1: Standard $k - \epsilon$ turbulence model constants

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
<th>$C_{\epsilon 1}$</th>
<th>$C_{\epsilon 2}$</th>
<th>$C_{\epsilon 3}$</th>
<th>$C_{\epsilon 4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.0</td>
<td>1.22</td>
<td>1.44</td>
<td>1.92</td>
<td>1.44</td>
<td>-0.33</td>
</tr>
</tbody>
</table>

compressibility effects.

In equation (2.25), the first term on the righthand side denotes the production of dissipation due to the shear stresses and compressibility effects, the third and fourth terms are also contributors to the production due to buoyancy and temporal density changes, whereas the second term is for the destruction of dissipation.

### 2.2.2 Spray modeling

The terms $\bar{S}_m$, $\bar{S}_f$, $\bar{S}_h$ and $\bar{S}_k$ in equation (2.12 - 2.15) are introduced due to the liquid spray (i.e., dispersed phase) interaction with continuous (i.e., gaseous phase) flow. In this thesis, the multi-phase interaction is modeled using a Lagrangian-Eularian approach as it is implemented in STAR-CD framework. In principle, the Lagrangian system of conservation equations for mass, momentum and energy for each individual droplet should be solved separately. The net rates for mass, momentum and energy exchange will define the additional source/sink terms for the continuous flow. Since the number of droplets is very high in a typical diesel engine spray, in order to reduce the computational cost only a finite number of parcels (with each parcel consisting of droplets having the same properties) is considered for computations. However, it is to be noted here that the term 'droplet' is used as general notation instead of 'parcels'. The conservation equations for the dispersed phase in the Lagrangian framework are described now.

The droplet mass transfer rate equation reads,

$$\frac{dm_d}{dt} = -A_s K_g p_t \ln \left( \frac{p_t - p_{\nu,\infty}}{p_t - p_{\nu,s}} \right),$$

(2.26)

where $A_s$ is the droplet surface area, $K_g$ is the mass transfer coefficient. $p_t$, $p_{\nu,\infty}$ and $p_{\nu,s}$ are the gas pressure, partial pressure of the vapor in the droplet surroundings and at its surface, respectively.

The droplet momentum transfer rate equation is given by,

$$m_d \frac{du_d}{dt} = \frac{1}{2} C_d \rho A_d |u - u_d|(u - u_d) - V_d \frac{\partial p}{\partial x} - C_{am} \rho V_d \frac{d(u_d - u)}{dt} + m_d g,$$

(2.27)

where, $u$ and $u_d$ are referred to as the velocity of the instantaneous gas flow and droplet. The terms on the right hand side of the above equation represents the drag, pressure, virtual mass and general body force due to gravity and acceleration, respectively. Hence, $C_d$ refers to
the drag and $A_d$ to the droplet cross-sectional area, $V_d$ is the droplet volume and $p$ is the static pressure of the fluid. $C_{am}$ is the virtual mass coefficient and $g$ is the gravitational acceleration.

The droplet energy balance equation is formulated as,

$$m_d c_{p,d} \frac{dT_d}{dt} = -A_s h(T_d - T) + h_{fg} \frac{dm_d}{dt},$$  \hspace{1cm} (2.28)

where, $T_d$ is droplet surface temperature. $c_{p,d}$ is the droplet specific heat. The terms on the righthand side are the droplet surface heat flux and latent heat due to phase change, respectively. And, $h$ is the heat transfer coefficient, while $h_{fg}$ is the latent heat.

The sum of the above mass, momentum and energy transfer rates from all droplets in the Lagrangian model at each cell provides, with an opposite sign, the additional source/sink terms to the continuous phase. For instance, the total momentum exchange rate for a group of droplets traversing a cell during time period $\Delta t = n_d \delta t_d$ reads,

$$\Delta M_d = \frac{1}{n_d} \sum_{\text{all droplets}} \sum_{n_d} \left( m_d \frac{u_d^n - u_d^o}{\delta t_d} \right),$$ \hspace{1cm} (2.29)

where, $\delta t_d$ is the parcel time step, $n_d$ is the number of parcels time steps. $n$ and $o$ denote ‘new’ and ‘old’ values during the parcel time step, respectively. This summation, with an opposite sign, will serve as the source terms $\tilde{S}_f$, in the momentum equation (2.13). Similarly the mass, energy and species (fuel vapor) exchange rates are integrated for each cell and incorporated as sources $\tilde{S}_m$, $\tilde{S}_h$, and $\tilde{S}_k$ to the respective conservation equations. The direct effects of the discrete phase on the turbulent flow of continuous phase are neglected.

**Figure 2.1:** Schematic of various sub processes in spray formation [Merker et al., 2006].

Apart from interaction with the continuous phase also the interaction between droplets and most importantly their formation needs to be described/modelled. Spray formation, after the injection of liquid fuel in continuous gas phase, occurs through many sub processes as depicted in Figure 2.1. Due to high injection pressures, in diesel engine the spray is considered to be characterized by the so-called atomization regime in which the liquid break-up starts
immediately after the injection hole. The major sub-processes include nozzle flow, primary breakup, secondary breakup, and other interactions such as evaporation, droplet collision and coalescence, wall interaction, turbulent dispersion, etc. These phenomena are included using dedicated sub models in STAR-CD which are described in detail now.

**Nozzle flow modeling**

The nozzle flow models are used to estimate the injection velocities at the exit of the nozzle. Accurate calculations of velocities are crucial as they strongly influence atomization, breakup and other subsequent processes. The three different models available in STAR-CD are the effective model, the MPI model [Obermeier, 1991] and the Modified MPI model [Obermeier, 1991 Gosman and Marooney, 1991]. MPI refers for the Max Planck Institute where the models are developed. The Modified MPI model is the most advanced model, which is used in this thesis.

![Figure 2.2: (a)Schematic of the Nozzle geometry for the MPI model. (b)Schematic of the boundary and cavitation layer development for the Modified MPI model.](image)

In this Modified MPI model, the actual injection velocity, $u_{ch}$, is expressed as

$$u_{ch} = \frac{4\dot{Q}}{r_{ch}\pi D^2},$$  

(2.30)

in which $\dot{Q}$ is the volume flow rate, $D$ is the nozzle diameter at exit and $r_{ch}$ the contraction ratio which is the ratio of the actual jet cross-section area at the nozzle and the geometrical section area. The reduction in area is due to obstruction by vapor which is created due to cavitation. This cavitation occurs because of the abrupt reduction in static pressure below the vapor pressure at a sudden flow transition.

The criteria used to check the occurrence of cavitation are based on the pressure in the chamber, $p_{ch}$, relative to the critical pressure in the chamber $p_{ch,crit}$ and it distinguishes three flow regimes in the nozzle hole:

1. Non-cavitating flow, $p_{ch} > p_{ch,crit}$: $r_{ch} = 1$
2. Cavitating flow where cavitation ends inside the nozzle $p_{ch} \leq p_{ch, crit} : r_{ch} = 1$

3. Cavitating flow where cavitation reaches the nozzle exit $p_{ch} \leq p_{ch, crit} : r_{ch} < 1$

The critical pressure is estimated using,

$$p_{ch, crit} = \rho_d \left\{ r_c u_c^2 - \left[ r_{ch} + \lambda \left( \frac{L}{D} - 1 \right) \right] \left( \frac{\dot{Q}}{A_o} \right)^2 \right\}, \quad (2.31)$$

Here, $\rho_d$ is the liquid fuel density, $r_c (= A_c/A_o)$ is the entrance contraction ratio where $A_c$ is the net cross section area as shown in Figure 2.2(a) and $A_o$ is the geometrical cross section area. $u_c (= \dot{Q}/(r_c A_o))$ is the velocity at the maximum contraction location. $L$ is the nozzle hole length, and $\lambda$ is the friction factor.

The expression used for $r_{ch}$ is :

$$r_{ch} = \frac{r_c^2 u_c^2}{u_c^2 \left\{ \frac{49}{72} + \frac{7}{36} \bar{R}_\rho (L) + \frac{1}{8} \bar{R}_\rho^2 (L) - \bar{R}_{cav}^2 (L) \right\} \frac{p_{ch}}{\rho_d}}, \quad (2.32)$$

where $\bar{R}_\rho$ is the boundary layer and $\bar{R}_{cav}$ is the cavitation layer thickness as shown in Figure 2.2(b).

### Primary breakup (or Atomization) modeling

The primary breakup of the liquid injected with high velocities is modeled using a so-called Atomization model. The main parameters of interest here are the break-up rate and the distribution of droplet size and velocities. The four models that are supported in STAR-CD are: Huh’s model [Huh and Gosman, 1991], the Reitz-Diwakar model [Reitz and Diwakar, 1986], the MPI model [Obermeier and Chaves, 1992] and the Modified MPI model [Obermeier, 1993].

In Huh’s model, the atomization process is mainly caused by the internal turbulence created by the nozzle flow and the inertia of the surrounded gas. The model estimates the initial perturbations created at the time of jet exit from the nozzle hole, and uses the surface wave growth theory, first to calculate the break-up rate, the spray angle, and then the initial velocities. The complete details can be found in [Sta, 2008]. The break-up rate is determined by,

$$\frac{dD_d}{dt} = - \frac{2L_A}{\tau_A \times 0.1}, \quad (2.33)$$

and the spray semi-cone angle is calculated using,

$$\tan(\beta) = \frac{L_A}{\tau_A U}, \quad (2.34)$$
where $L_A$, $\tau_A$ are known as atomization length and time scales, respectively. These are functions of turbulence length and time scales (along with wave growth time scales) which are derived by turbulence calculations at the nozzle exit. $U$ is the average injection velocity. The spray semi cone angle ($\beta$) is used to estimate the magnitude of initial velocities using the expression, $u_d \sim U_{ch} \sin(\beta)$.

In the Reitz-Diwakar model, the initial velocity is determined in a similar way as in Huh’s model, however the spray cone angle has to be provided as an user input parameter. The important thing to note here is that the Reitz-Diwakar models for atomization and (secondary) droplet breakup are based on the same hypothesis so the Reitz-Diwakar atomization model should only be applied in combination with the Reitz-Diwakar droplet break-up model in STAR-CD. The details of the model are discussed in Section 2.2.2.

**Figure 2.3**: Schematic for (a) MPI atomization model. (b) Modified MPI atomization model.

In the MPI models, a chain of primary droplets with an initial diameter equal to the nozzle diameter are considered to represent the initial liquid core. During the atomization process due to the aerodynamic forces, they break into secondary droplets over the length of the liquid core. The main differences between the MPI and modified MPI model are, firstly, the interpretation of the liquid core length $L_c$ which is illustrated in Figure 2.3(a) for the MPI, and in Figure 2.3 b) for the Modified MPI, respectively. Secondly, the change in the diameter of the primary drops as a function of $x$ is given by,

$$D_d = \sqrt{(D_c^2 - D^2) \left( \frac{x}{L_c} \right) + D^2}$$ \hspace{1cm} (2.35)

in case of MPI and,

$$D_d = D - (D - D_c) \frac{x}{L_c}$$ \hspace{1cm} (2.36)

in case of Modified MPI model. Here, $D_c$ is the diameter at the tip of the core and $D$ is nozzle diameter. $L_c$ is expressed as,

$$L_c = CD \sqrt{\frac{\rho d}{\rho}},$$ \hspace{1cm} (2.37)
in which $\rho_d$ and $\rho$ are the densities of droplet and gas phase, respectively. $C$ is an empirical constant, and equals 7.0 for MPI and 4.0 for the modified MPI model.

Secondary (or Droplet) breakup modeling

After primary breakup, the droplets become unstable due to the interfacial forces caused by the high relative velocities between droplet and gas phase. They continue to breakup into smaller droplets. The process is called Secondary (or droplet) breakup. The three droplet breakup models available in STAR-CD to model this phenomenon are: (1) the Reitz-Diwakar model [Reitz and Diwakar, 1986], (2) the Pilch and Erdman model [Pilch and Erdman, 1987] and (3) the Hsiang and Faeth model [Hsiang and Faeth, 1992]. The expression used for the change droplet diameter is:

$$\frac{dD_d}{dt} = -\frac{(D_d - D_{d,stable})}{\tau_b},$$

(2.38)

where $D_d$ is the instantaneous droplet diameter, $D_{d,stable}$ is the stable diameter, and $\tau_b$ is the breakup timescales. The important dimensionless parameter used by these models for defining criteria for breakup occurrence is the Weber number ($We$), which is the ratio between the inertial forces and the surface tension:

$$We = \frac{\rho_g |u - u_d|^2 D_d}{\sigma_d}.$$  

(2.39)

Here, $\rho_g$ is the gas density and $\sigma_d$ is droplet surface tension.

The models are distinguished based on the way they consider the regimes for breakup occurrence (mainly on the basis of Weber number), and the correlation used for calculating breakup timescales ($\tau_b$) and stable diameter ($D_{d,stable}$). Different droplet break-up regimes and the Weber number criteria can be found in [Wierzba, 1990]. In the Reitz Diwakar model, break-up occurs in so-called Bag and Stripping break-up modes, whereas in the Pilch and Erdman model, it occurs in vibrational, bag, bag/steamer, sheet stripping, and wave crest stripping breakup modes. In Hsiang and Faeth model, break-up happens only if $We > 12$. The other criterion for break-up modes and correlations for timescales and stable diameter is provided in [Sta, 2008]. For simplicity, only the details of Reitz-Diwakar model are presented in Table 2.2.

Other spray interaction phenomena modeling

In this section, the models used for other interactions are stated briefly. The turbulence dispersion effect on random velocities of a droplet is taken into account using a standard model in STAR-CD which is based on a stochastic approach using a Gaussian probability density functions. The model of O'Rourke [O'Rourke, 1981] is used to model the inter-droplet collisions, while Bai’s spray impingement model [Bai and Gosman, 1995] is used to account the droplet and wall interactions. The evaporation of droplets is accounted by using
Table 2.2: Reitz-Diwakar droplet break up model

<table>
<thead>
<tr>
<th>Break-up mode</th>
<th>Criterion</th>
<th>Break-up timescale</th>
<th>Stable diameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bag break-up</td>
<td>$We \geq 12$</td>
<td>$\tau_b = \frac{\pi \rho_d \frac{5}{2} D_d \frac{3}{2}}{4 \sigma_d \frac{3}{2}}$</td>
<td>$D_{stable_d} = \frac{\sigma_d^2}{\rho_d^2</td>
</tr>
<tr>
<td>Stripping break-up</td>
<td>$We \geq 0.5 \sqrt{Re_d}$, $Re_d$ is droplet Reynolds number</td>
<td>$\tau_b = \frac{20}{2} \left( \frac{\rho_d}{\rho} \right) \frac{1}{2} \frac{D_d}{</td>
<td>u-u_d</td>
</tr>
</tbody>
</table>

standard boiling models where it covers the situations when the droplet reaches the boiling or critical temperatures. The heat and mass transfer coefficients are estimated using Ranz-Marshall correlations [Ranz and Marshall, 1952], while the drag coefficient is calculated using standard correlations in STAR-CD [Sta, 2008].

### 2.3 Combustion modeling - FGM

In this thesis, the Flamelet Generated Manifold (FGM) is applied for combustion modeling. FGM is based on the same philosophy as the flamelet approach where it is assumed that locally a (turbulent) flame can be described by a representative 1D flame (a flamelet). The stiffness and computational effort can then be significantly decreased by decoupling the detailed kinetics from the flow simulation. The detailed kinetics are pre-computed for relevant 1D flames and their solutions are tabulated. The difference with the classical flamelet approach lies in the tabulation procedure and the subsequent application of the tabulation in the flow solver. The tabulation procedure in FGM bares a great resemblance with that applied in ILDM. Instead of the mixture fraction and the scalar dissipation, here the mixture fraction and controlling variables are used to create the look-up tables. FGM method was first developed [van Oijen, 2002] and applied for various combustion systems with premixed, non-premixed [Vreman et al., 2009] and partially premixed [Bongers, 2005 Ramaekers, 2011] configurations.

The fundamental aspect of FGM for any application is coupling of the pre-tabulated chemistry database to the online turbulent flow (CFD) simulations. However, the main features that characterize the FGM for a specific application are the configurations used for the representative laminar flames, an appropriate parametrization of the chemistry and the treatment of turbulent-chemistry interaction. In this section, these aspects specific to diesel combustion are defined and explained in-details followed by a description of the implementation.
2.3.1 The canonical configurations

Since the computation of the chemistry is decoupled from the real-time simulations, the selection of relevant configurations for the generation of the chemistry database is important and application dependent. In diesel combustion, the conventional combustion mode is dominated by non-premixed flames whereas the early injection combustion mode is well represented by well-mixed or near-homogeneous ignition. Hence, the two configurations selected in this thesis are the Igniting Counterflow Diffusion Flames and the Homogeneous Reactors which are described further-on.

Igniting Counterflow Diffusion Flames (ICDF)

The counterflow setup is one of the standard setups for generating 1D flames. The oxidizer and fuel streams are two opposing streams and react in a thin region close to the stagnation plane. These flames are commonly referred to as counterflow diffusion flames. Here the term Igniting is added to indicate the explicit inclusion of the transient behavior to incorporate the auto-ignition process. The schematic of a counterflow setup with a diffusion flame is as shown in Figure 2.4

![Schematic for counterflow setup.](image)

The governing equations for a 1D igniting counterflow diffusion flame can be derived from equations (2.1 to 2.3, 2.5), and read [Stahl and Warnatz, 1991]:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = -\rho G,  
\]

\[
\frac{\partial (\rho h)}{\partial t} + \frac{\partial}{\partial x}(\rho uh) = \frac{\partial}{\partial x} \left[ \frac{\lambda}{c_p} \frac{\partial h}{\partial x} + \lambda \sum_{k=1}^{N_s} \left( \frac{1}{L e_k} - 1 \right) h_k \frac{\partial Y_k}{\partial x} \right] - \rho G h,  
\]

\[
\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial}{\partial x}(\rho u Y_k) = \frac{\partial}{\partial x} \left( \frac{\lambda}{L e_k c_p} \frac{\partial Y_k}{\partial x} \right) + \dot{\omega}_k - \rho G Y_k \quad k \in [1, N_s],  
\]
\begin{equation}
\rho \frac{\partial G}{\partial t} + \rho u \frac{\partial G}{\partial x} = \frac{\partial}{\partial x} (\mu \frac{\partial G}{\partial x}) - \rho G^2 + \rho_{ox} a^2, \tag{2.43}
\end{equation}

where $Le_k$ is the Lewis number of species $k$, and is assumed here to be equal to one. This assumption is widely used and it simplifies the above transport equations to a great extent. $\lambda$ and $c_p$ are the heat conductivity and specific heat of mixture, respectively.

The local flame stretch rate $G = \frac{\partial u}{\partial y}$ is introduced in the counterflow setup to define the $y$-component of the flow. $G$ is a function of the $x$-coordinate and time and varies by the applied strain rate ($a$) at the oxidizer boundary. The boundary conditions for $G$ are: $G(x \to -\infty) = a$, $\frac{\partial G}{\partial x}(x \to \infty) = 0$, thus the only parameter to describe the influence of the external flow field on the 1D flamelets is due to $G$ which, in return is defined by the strain rate, $a$.

The boundary conditions for $Y_k$ and $h$ are imposed on both oxidizer ($x \to -\infty$) and fuel ($x \to \infty$) stream sides as given below,

\begin{equation}
Y_k(x \to -\infty) = Y_{i,ox}, \quad h(x \to -\infty) = h_{ox}, \tag{2.44}
\end{equation}

\begin{equation}
Y_k(x \to \infty) = Y_{i,fu}, \quad h(x \to -\infty) = h_{fu}. \tag{2.45}
\end{equation}

The oxidizer stream can be pure air or a mixture of air and combustion products to represent a non-EGR or EGR conditions, respectively. Whereas, pure fuel is considered as the fuel stream throughout the thesis. A dedicated 1D flamelet code i.e., CHEM1D which is developed at Eindhoven University of Technology [Somers, 1994 CHEM1D, 2012] is used to generate the laminar counterflow flames. The initial conditions for igniting counterflow flames is provided by a frozen solution which is a pure mixing line at the prescribed condition (pressure, fuel & oxidizer temperature and strain rate). To illustrate an igniting counterflow flame structure, the temperature and reactants evolution in time are shown in Figure 2.5 for a typical case that is studied in this thesis: $T_{fu} = 363$ K, $T_{ox} = 900$ K, $p = 60.0$ MPa, applied strain rate, $a = 500$ s$^{-1}$. The diesel surrogate fuel i.e., $n$-dodecane and oxidizer (diluted with EGR) are used as streams. The red lines indicates the initial solution and the green line shows the steady solution (as $t \to \infty$). It should be noted that the complete computational domain (i.e., from -0.1 cm to +0.1 cm) is not shown, only the flame region is given.

**Homogeneous Reactors (HR)**

The homogeneous reactor is a simplified zero-dimensional reactive systems. It can not account for the convection and diffusion, which is the fundamental difference with the ICDF. Hence, the governing equations for the HR are obtained by eliminating the terms associated with $x$-coordinates, $G$ and $a$ from equations (2.40 - 2.43). We have for the mass conservation law:
Figure 2.5: Species mass fractions, and Temperature as a function of spatial co-ordinates, in an Igniting Counterflow Diffusion Flame. The vertical dotted line indicates the stagnation plane. The arrow indicates the time evolution.

\[ \frac{\partial \rho Y_k}{\partial t} = \omega_k, \quad k \in [1, N_s], \quad (2.46) \]

and for the energy conservation law,

\[ \frac{\partial \rho h}{\partial t} = 0. \quad (2.47) \]

At a given mixture composition, the equilibrium state is arrived as \( t \to \infty \). The homogeneous reactor simulations are performed using an in-house developed code based on the DASSL code.

### 2.3.2 Parametrization

The full chemical composition space of the above solutions can be represented in a \( N_s \) dimensional space, \( N_s \) being number of species. The philosophy of the FGM approach (and ILDM for that matter) is now that the path of the chemical conversion of the initial...
state to the final state is essentially captured by a low dimensional manifold in composition space. This manifold can effectively be 'parametrized' by a few so-called controlling variables. An increase in number of controlling variables (up to $N_s$) will increase the accuracy at the cost of computational effort needed to solve the transport equations for the controlling variables in the flow solver and a more complex look-up procedure. In this thesis, two controlling variables are used: (1) Mixture Fraction ($Z$) and, (2) Progress Variable ($\mathcal{Y}$).

The mixture fraction is defined based on local element compositions. The well-known definition of Bilger [Bilger et al., 1990] is applied,

$$Z = \frac{2Y_C^e - Y_{C,2}^e}{M_C} + 0.5 \frac{Y_H^e - Y_{H,2}^e}{M_H} - \frac{Y_O^e - Y_{O,2}^e}{M_O},$$

(2.48)

where $Y_i^e$ is the element mass fraction and $M_i^e$ is the molar mass of the elements. The subscripts C, H, O refer to the carbon, hydrogen and oxygen elements, respectively. The subscripts 1 and 2 refer to the constant mass fraction in the defined fuel and oxidizer stream, respectively. Hence, $Z = 1$ at the fuel stream and $Z = 0$ at the oxidizer stream.

The progress variable is defined based on a combination of species which describes the reaction progress from the unburnt mixture to chemical equilibrium. The main prerequisite is that it has to increase or decrease in time monotonically. In this study, weighted mass fractions of carbon dioxide ($CO_2$), carbon monoxide ($CO$) and hydroperoxyl ($HO_2$) are chosen resulting in the following definition of $\mathcal{Y}$:

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

(2.49)

$Y_i$ and $M_i$ are the mass fraction and molar mass of species $i$, respectively. The inclusion of $HO_2$ is inspired by the notion that it is significant at the start of the ignition process, $CO$ represents the intermediate stage and subsequently ends with $CO_2$. It is to be noted here that the definition of progress variable ($\mathcal{Y}$) will not affect results as long as the chemistry parametrization (selection of species) represents each stage of chemistry evolution and is monotonic.

Using these two variables, the flame solutions in space and time coordinates are transformed to low dimensional manifolds. To illustrate this, the solutions are plotted in Figure 2.6 as a function of $Z$. The co-ordinate transformation from spatial to $Z$ space reduces the steep gradients within the thin regions, which improves the interpolation process.

2.3.3 Turbulence chemistry interaction (TCI)

The parametrized laminar chemistry data (referred to as the laminar table) formally cannot be coupled directly to the turbulent flow calculations. The transport equations that are solved in a RANS setting describe the evolution of the average quantities for each variable. Consequently averaged quantities need to be communicated from the table to the solver. For instance, the transport equation for $\tilde{\mathcal{Y}}$ needs $\tilde{\mathcal{Y}}$ which is not equal to $\tilde{\mathcal{Y}}(\tilde{Z}, \tilde{\mathcal{Y}})$. Hence, TCI is
a way to compute $\tilde{\gamma}$. Many approaches exist to perform TCI such as transported/presumed pdf methods [Kung and Haworth, 2008], CMC method [Wright et al., 2009], characteristic timescales approach [Abraham et al., 1985], etc.

In this thesis, the presumed pdf approach is used to integrate the laminar table in order to account for the effect of turbulent fluctuations. The presumed pdf approach is widely used and is computationally less expensive compared to transported pdf methods. The quantities in the laminar table are integrated with a $\beta$-PDF that is a function of the means and variances of $Z$, $Y$ variables.

When $Z$ and $Y$ are assumed statistically independent, the mean quantities are defined as,

$$\tilde{f}(\tilde{Z}, \tilde{Z}''^2, \tilde{Y}, \tilde{Y}''^2) = \int_0^1 \int_0^1 f(Z, Y) P(Z \parallel \tilde{Z}, \tilde{Z}''^2) P(Y \parallel \tilde{Y}, \tilde{Y}''^2) dZdY, \quad (2.50)$$

It is also important to note here that $Y$ is scaled between 0 and 1, prior to pdf integration, to render the statistical independent relation between $Z$, $Y$.
So far, the details of the characterizations of FGM for diesel combustion applications are described. In the next section, the entire scheme for implementation of FGM in the CFD code for modeling diesel spray combustion is presented.

### 2.3.4 Implementation of FGM

![Figure 2.7: Schematic for preprocessing of FGM and coupling to CFD solver](image)

The implementation procedure of FGM in a CFD solver consists of two parts as shown in Figure 2.7. The first part is preprocessing of the chemistry database and the other is coupling of the database to online CFD simulations. The preprocessing step is carried out, as explained in earlier Sections (2.3.1 - 2.3.3). Hence it can be seen as three systematic steps. In first step, the raw chemistry data is generated in space and time using ICDF configuration or only in time using HR configuration. Then, in next step, the co-ordinate transformation is performed to generate 2D tables using $Z$, $Y$ as controlling variables. In ICDF, both igniting and stationary flames are included to cover the entire $(Z, Y)$ regime of diesel combustion. The igniting flame generated at a single strain rate, is tracked to capture the ignition until a steady state solution is reached. This table is completed with a set of stationary flames applying varying strain rates. Lower strain rate solutions approach chemical equilibrium. Figure 2.8 gives the complete illustration of a typical dataset generated using ICDF’s at prescribed conditions. For the HR-based tables a series of HR’s are simulated spanning the composition space from $Z = 0$ to $1$. The initial conditions are obtained from the frozen chemistry adiabatic mixing limit, identical to the initial composition specified for the ICDF as illustrated in Figure 2.8. The solution starts from initial mixing conditions and reaches equilibrium as $t \to \infty$. Finally, in the last step of the preprocessing, the 2D laminar data is
pdf integrated to generate 4D tables including variances $\tilde{Z}, \tilde{Z}^{\prime\prime}, \tilde{Y}$ and $\tilde{Y}^{\prime\prime}$.

**Figure 2.8:** Typical subspace of Mixture Fraction and Progress variable for both ICDF and HR approaches. For ICDF, the green lines show the evolution of ignition flames in time and blue lines show the stationary flames are varying strain rate. For HR, the red arrows indicates the discrete cases at each mixture fractions conditions.

In the second part of the implementation process, the preprocessed FGM table is coupled to the online flow calculations in the CFD solver. STAR-CD is used to solve RANS equations for turbulent flow and spray formation. In order to enable the coupling, transport equations are embedded in the CFD solver for the controlling variables next to the standard mass, momentum and energy equations. The transport equations for $\tilde{Z}, \tilde{Y}, \tilde{Z}^{\prime\prime}, \tilde{Y}^{\prime\prime}$ read,

$$
\frac{\partial}{\partial t}(\tilde{Z}) + \frac{\partial}{\partial x_i}(\tilde{\rho} u_i \tilde{Z}) - \frac{\partial}{\partial x_i} \left[ \tilde{\rho} (D + D_T) \frac{\partial \tilde{Z}}{\partial x_i} \right] = \tilde{Z}_{spray}, \quad (2.51)
$$

$$
\frac{\partial}{\partial t}(\tilde{Y}) + \frac{\partial}{\partial x_i}(\tilde{\rho} u_i \tilde{Y}) - \frac{\partial}{\partial x_i} \left[ \tilde{\rho} (D + D_T) \frac{\partial \tilde{Y}}{\partial x_i} \right] = \tilde{Y}, \quad (2.52)
$$

$$
\frac{\partial}{\partial t}(\tilde{Z}^{\prime\prime}) + \frac{\partial}{\partial x_i}(\tilde{\rho} u_i \tilde{Z}^{\prime\prime}) - \frac{\partial}{\partial x_i} \left[ \tilde{\rho} (D + D_T) \frac{\partial \tilde{Z}^{\prime\prime}}{\partial x_i} \right] =
2\tilde{\rho} \left[ D_T \left( \frac{\partial \tilde{Z}}{\partial x_i} \right)^2 - \frac{\varepsilon}{\kappa} \tilde{Z}^{\prime\prime} \right], \quad (2.53)
$$
\[
\frac{\partial}{\partial t} (\bar{\rho} \overline{\dot{Y}^m}^2) + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \overline{Y}^m) - \frac{\partial}{\partial x_i} \left[ \frac{\partial}{\partial x_i} \left( \bar{\rho} (D + D_T) \frac{\partial \overline{Y}^m}{\partial x_i} \right) \right] = \\
2\bar{\rho} \left[ D_T \left( \frac{\partial \tilde{Y}^m}{\partial x_i} \right)^2 - \frac{\varepsilon}{\kappa} \overline{Y}^m \right] + 2 \overline{\dot{Y}^m \dot{Y}^m}.
\] (2.54)

The \(\tilde{Y}, \overline{Y}^m \tilde{Y}\) terms are retrieved from the FGM database during the CFD simulation.

**2.4 Summary and outlook**

To summarize, the basic numerical methodology used in this thesis for modeling diesel spray combustion is presented. The generic conservation equations for reacting flows and some details of chemical kinetics are described briefly. Since diesel spray combustion is characterized by a spray induced turbulent auto-igniting combustion event, the multidimensional modeling of all processes and their interaction poses various challenges. The RANS formulation of the conservation equations for turbulent spray combustion is described along with the additional terms due to turbulence averaging, and spray interaction. Then, the existing sub models for turbulence (based on eddy viscosity approach) and spray formation (using stochastic Lagrangian-Eularian model) from the specific CFD solver used here have been summarized. Subsequently, the main method implemented to solve combustion problems i.e., the Flamelet Generated Manifold is introduced in a systematic way. First, the individual aspects of FGM generation are described. It includes introducing two canonical configurations i.e., ICDF and HR that are considered to generate the raw chemistry data, the parametrization of chemistry via two controlling variables i.e., mixture fraction and progress variable and the turbulence closures applied based on the presumed pdf integration. Finally, the complete implementation i.e., generation of FGM and coupling with CFD solver is presented.

The FGM methodology along with the turbulence and spray models is applied to model both non-reacting and reacting diesel sprays in a constant volume combustion chamber and model enhancements are studied systematically, in the next chapter. Further, the methodology is extended to model combustion in a moving piston geometry for engine cycle simulations by incorporating more dimensions in the FGM tables. This study is included in Chapter 4. In the subsequent chapter, the soot model is added to the FGM methodology to predict the formation and oxidation of soot using detailed chemistry.
Chapter 3

FGM approach for Igniting Diesel Spray characteristics

This work is carried out by the collaborative efforts of the author and his colleague U. Eğüz. Mainly, the author is responsible for ICDF based FGM simulations; while U. Eğüz performed HR based FGM simulations. The content is extracted from the following publications.


3.1 Introduction

The combustion process in diesel engines is initiated by the auto-ignition event of a pressurized liquid fuel introduced into a compressed turbulent gas. Understanding and achieving better control of this key phenomenon is important for optimizing the engine performance and reducing emissions. Hence, characterization of the diesel ignition process has become an active research topic since a number of years. In order to predict this vital phenomenon accurately to aid industrial engine research, there is a need for efficient combustion models. However, the modeling of an igniting high pressure spray involves modeling of many complex physical and chemical processes starting from break-up, atomization, and evaporation.
of a dense liquid spray, turbulent mixing of the fuel with the hot ambient air and most importantly the ignition event. The nonlinear characteristics of the auto-ignition process of a heavy hydrocarbon fuel involves a huge set of species with many chemical pathways, furthermore the interaction between turbulence and chemistry in practical applications makes it impossible to use detailed chemical mechanisms in direct numerical simulations. However incorporating detailed chemistry effects induced by the intermediate species is essential for the model to capture the fuel effects and the sensitivities due to the varying in-cylinder conditions. To address this, reduction methods are reported in literature which can be majorly classified as chemical reduction models [Peters, 1991 Smith et al., 2012], or mathematical reductions models [Maas and Pope, 1992 Lam and Goussis, 1994].

The Flamelet Generated Manifold (FGM) method is an efficient tabulated chemistry approach [van Oijen, 2002] to model turbulent reacting flows capturing the effects of detailed chemistry. The FGM method, in a nutshell, combines advantages of (i) the laminar flamelet concept [Peters, 1984] which assumes that a turbulent flame can be considered as an ensemble of thin laminar flamelets since the chemical reaction timescales are significantly shorter than the turbulent timescales and hence the reaction zone is not disturbed by turbulent eddies; and (ii) the Intrinsic Low Dimensional Manifold (ILDM) approach [Maas and Pope, 1992], where the chemical system is reduced by assuming that fast processes are frozen. The first implementation of FGM to diesel spray combustion modeling using n-heptane [Bekdemir et al., 2010] at one single operating condition was successful. In the method, 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. For extensive validation of computational models, well-documented experimental data is also required. For that purpose, the Engine Combustion Network (ECN) is formed by a number of international experimental and computational groups, with the purpose to generate a high quality standard experimental database [ECN, 2012] at engine-like conditions. The controlled experiments are performed in a constant volume combustion vessel with a single igniting spray under varying operating conditions. Spray H and Spray A are sprays of n-heptane and n-dodecane diesel surrogate fuels, respectively. Recently, the diesel combustion fraternity is more attracted to n-dodecane due to the fact that n-dodecane is easier to handle and cheaper when compared to n-heptane while being closer to diesel’s C/H ratio and cetane number. The engine research team of the Combustion Technology (CT) group at Eindhoven University of Technology (TU/e) is contributing actively to this network by both experimental and modeling work. With the advent of ECN, it is intended to use the wide set of experimental data for FGM model improvement.

The objective of the current study is to evaluate and enhance the ignition predictability of FGM and to validate the model at various ‘engine like’ operating conditions. The optimal implementation of the model is determined at various stages. Although the main focus is on combustion modeling, first the sensitivities of the CFD model settings from the STAR-CD solver for spray formation are evaluated to achieve the best combination. This is performed using both Spray H and Spray A non-reacting conditions. Then, these optimum CFD model settings are used to implement FGM and model the ignition behavior as function of ambient gas $O_2$-concentration, for Spray H conditions. The performance of FGM which is a tabulated chemistry method depends on the quality of the interpolation from the database. So it
is intended to perform a table resolution study to determine an adequate table size to capture the ignition accurately. The effect of two different table generation methods, i.e. canonical systems namely Igniting Counter flow Diffusion Flames (ICDF) and Homogeneous Reactors (HR) is included in this study. Finally, to test the robustness of the FGM model approach, the model is applied to a parametric sweep of Spray A using detailed chemistry of \( n \)-dodecane. This parametric sweep consists of variations in \( O_2 \), ambient temperature, ambient density, and injection pressure so as to represent the Exhaust Gas Recirculation (EGR) change, crossing Low Temperature Combustion (LTC) zones, higher boost and rail injection pressure conditions that occur in real engines, respectively. The results are compared with the measurements to assess the ability of the model to capture the sensitivities with respect to the change in conditions.

In the following sections, first the non-reacting spray modeling studies are presented. Further, the FGM methodology is explained along with the chemistry table generation approach. Then, the combustion modeling studies are presented which comprises an a-priori, table resolution and TCI studies with Spray H cases and detailed parametric studies with Spray A cases.

### 3.2 Non-reacting spray modeling

Modeling spray formation accurately is an essential prerequisite to model the combustion event in a more reliable way. The Lagrangian two phase spray models and in-built turbulence models from STAR-CD (CFD solver) are used to model non-reacting and the turbulent flow field, respectively. A detailed explanation of these models is given in Section 2.2 of Chapter 2. However, a selection of the best combination of model settings is required to capture the spray formation as accurately as possible. Hence in this current section, a sensitivity study is performed with respect to the model settings. Firstly, the model settings along with the operating conditions of the non-reacting cases are given. And then, spray results are compared with well documented results [ECN, 2012] and best combination of these model settings are deduced for use in the reacting spray modeling.

#### 3.2.1 Model settings

A uniform 3D mesh is created to define the computational domain for a constant volume chamber. The actual dimension of the cubical shaped combustion vessel in the experiments [ECN, 2012] is 108 mm on each side. However, the dimensions of the domain (40 mm X 40 mm X 100 mm) that being considered for modeling are adequate so as to avoid the influence of the boundary wall on the spray penetration. Further, to reduce the computational effort, a quarter (1/4\(^{th}\)) section of the domain is used by using symmetry planes (as shown in Figure 3.1).

The Eulerian - Lagrangian based spray model resolves the discrete phase (liquid) and continuous phase (gas) simultaneously. In order to avoid accuracy problems caused by a large fluid fraction, the following equation is used according to [O’Rourke, 1981], to determine the minimum size of the cell:
Table 3.1: Model settings

<table>
<thead>
<tr>
<th>Grid type</th>
<th>3D, uniform</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell width (mm)</td>
<td>0.25 - 0.5 - 1</td>
</tr>
<tr>
<td>Time step (µs)</td>
<td>1 - 10</td>
</tr>
<tr>
<td>(k-\epsilon) turbulence model</td>
<td>High Re - RNG - Realizable</td>
</tr>
<tr>
<td>Nozzle flow model</td>
<td>Modified MPI</td>
</tr>
<tr>
<td>Breakup model</td>
<td>Reitz-Diwakar, Pitch-Erdman, Hsiang-Faeth</td>
</tr>
<tr>
<td>Atomization model</td>
<td>Huh, Reitz-Diwakar, MPI, Modified MPI</td>
</tr>
<tr>
<td>Collision model</td>
<td>(O'Rourke)</td>
</tr>
<tr>
<td>Turbulence dispersion, Drag, Heat and mass Transfer</td>
<td>Standard correlations</td>
</tr>
</tbody>
</table>

\[
\frac{V_{cell} \cdot \rho_f}{\dot{m}_{fuel}} > 10^{-7}. \tag{3.1}
\]

\(V_{cell}\) is the cell volume, \(\rho_f\) is the fuel density and \(\dot{m}_{fuel}\) is the flow rate of fuel. The width of a cubic cell (i.e. with unit aspect ratio) should be larger than \(\sim 0.07 \text{ mm}\), for the operating conditions of a typical diesel spray. However, to achieve a practical computational time (with an adequate number of cells for a large domain) the minimum cell width is kept at 0.25 \(\text{mm}\). Other cell widths considered for this study are 0.5 \(\text{mm}\) and 1 \(\text{mm}\). The solver time step size has a major influence on the continuous phase calculations, which in turn influences the droplet behavior. In the previous study [Rijk, 2009], a size of 10 \(\mu\text{s}\) was considered to be sufficient for the time step. To study the sensitivity of the solution to the time step size, 1 \(\mu\text{s}\) is also used. In addition to the numerical parametric study, the effect of three variants of the \(k-\epsilon\) turbulence model (High Re, RNG, and Realizable) is investigated.

inside the nozzle on the flow exit velocity. Cavitation depends on the critical pressure inside the chamber. The subsequent droplet breakup process and interactions can be modeled using various sub-models. The primary breakup or atomization models differ in the way the droplet size distribution and initial velocities are calculated. Huh [Huh and Gosman, 1991], Reitz-Diwakar [Reitz and Diwakar, 1986], MPI [Obermeier and Chaves, 1992], Modified MPI [Obermeier, 1993] are the models tested in this study. The Weber number, which is the ratio of inertial to surface tension forces, determines the secondary breakup regime and the actual rate of breakup. The difference between the different available droplet breakup models is mainly related to the correlations that are used to estimate the time scale of the break-up process and the stable droplet diameter. Reitz-Diwakar [Reitz and Diwakar, 1986], Pitch-Erdman [Pilch and Erdman, 1987], Hsiang-Faeth [Hsiang and Faeth, 1992] models are considered in this study. The only precondition of using combinations of these sub-models is that the Reitz-Diwakar atomization model has to be used in conjunction with the Reitz-Diwakar droplet break-up model. The inter-droplet collisions causing coalescence, separation and bouncing are modeled using O’Rourke’s model [O’Rourke, 1981]. The other phenomena like turbulence dispersion, drag and heat and mass transfer (evaporation) are modeled using standard correlations in STAR-CD.

An overview of the model settings corresponding to numerical parameters, turbulence models and spray sub-models is given in Table 3.1. It should be noted that the simulations are performed with the default settings i.e. without tuning any constants/coefficients of any sub-models.

### 3.2.2 Spray model results

The models are applied for the non-reacting cases of Spray H and Spray A for which the corresponding operating conditions are presented in Table 3.2. The results for spray penetration length, liquid penetration length and mixture fraction field are compared with the experimental data. Here, the spray penetration length is defined as the farthest point from the nozzle exit where the mixture fraction exceeds 0.001, and the liquid penetration length is defined as the farthest location where the local liquid volume fraction exceeds 0.15%. The definitions are according to the proposals from the first ECN workshop [ECN, 2012].

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Spray H</th>
<th>Spray A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection rate (g/s)</td>
<td>2.69</td>
<td>2.40</td>
</tr>
<tr>
<td>Injection pressure (MPa)</td>
<td>150</td>
<td>150</td>
</tr>
<tr>
<td>Nozzle hole diameter (mm)</td>
<td>0.100</td>
<td>0.090</td>
</tr>
<tr>
<td>Ambient temperature (K)</td>
<td>1000</td>
<td>900</td>
</tr>
<tr>
<td>Ambient density (kg/m³)</td>
<td>14.8</td>
<td>22.8</td>
</tr>
<tr>
<td>Fuel temperature (K)</td>
<td>373</td>
<td>363</td>
</tr>
<tr>
<td>O₂ (%)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 3.2: Operating conditions of non-reacting cases.
Firstly, the effect of model settings, i.e. cell width, solver time step and turbulence models (Table 3.1) on the model’s result is assessed. Spray H conditions are applied for these studies and key observations are discussed here. In Figure 3.2 the evolution of spray penetration length (SL) in time is plotted for three different $k-\epsilon$ turbulence models, at two different solver time steps along with experimental data. For all cases, the cell width is kept at 0.5 mm and the atomization-breakup model used is Reitz-Diwakar. It is observed from the results that the standard high Re $k-\epsilon$ model matches well with the experimental data, for both time steps, up to 1.5 ms (60 mm). This is especially critical since the ignition for all reacting cases occurs typically within this range. The Realizable $k-\epsilon$ model under-predicts the penetration considerably and it is very sensitive to solver time step change. Finally, the RNG model over-predicts SL from the start which is due to the fact that it predicts a lower turbulent viscosity. Similar results are observed for different mesh size cases. Since the high Re $k-\epsilon$ model demonstrates a better match with the experiments for a range of time step sizes, it is applied for the rest of the study. Though 10 $\mu$s shows a slightly improved match with experimental data, in light of the reactive simulations, 1 $\mu$s is considered for the rest of the study.

Figure 3.3 illustrates the dependence on the grid size (with $\Delta t$ of 1 $\mu$s, $k-\epsilon$, high Re, and Reitz-Diwakar model) on resolving the mixture fraction field (left) and predicted liquid penetration lengths (right). The radial profile of mixture fraction at an axial distance of 17 mm from the nozzle hole, and at 0.47 ms time (around which ignition of the baseline case typically occurs) is compared with experimental data. It is noticeable that a 1 mm cell width is not sufficient to capture the radial distribution of the fuel. The deviation from experimental data decreases when the cell width is reduced to 0.5 mm however still underestimates the maximum value. The case with cell width of 0.25 mm resolves the flow field with spray more accurately and shows the best match with experimental data. However, the predicted liquid penetration length increases with decrease in cell size. The reason behind this effect is that the smaller cell results in higher vapor mass fractions, which leads to higher partial pressures of vapor. Due to this higher vapor pressure, the evaporation rate reduces [Bird
et al., 1966] and as a consequence the liquid penetration length is over-predicted. Since an accurate prediction of mixture fraction is more important than the liquid penetration length in the reacting case, a cell width of 0.25 mm is selected for further study.

Next, by keeping the above best model settings fixed (\(\Delta x, \Delta t\) and turbulence model), the effect of various spray sub-models on the predictions is studied. Many simulations with combinations of atomization and breakup models (as considered in Table 3.1) are carried out for the non-reacting case of Spray A. The operating conditions for Spray A are shown in Table 3.2. First, spray penetration results are compared with experimental data and the best cases are presented in Figure 3.4 (left). The notation for each model is RD (Reitz and Diwakar), PE (Pilch and Erdman), HF (Hsiang and Faeth), MPI (MPI) and MPI2 (Modified MPI). The RD atomization model is slightly over predicting at an early stage and under predicting at later stages. Other atomization models i.e. MPI and MPI2 predict the spray
penetration accurately until $t = 0.4 \text{ ms}$ and start deviating more from experimental data afterwards. Importantly, the change in droplet breakup models does not show much impact on spray penetration. Typical higher injection pressures of diesel sprays lead to atomization governed conditions hence the atomization models as they estimate the injection velocities and droplet distribution have a higher impact on spray penetration. In Figure 3.4(right), the liquid penetration lengths are plotted. Here, the droplet break-up models show considerable impact on the predictions. Except the PE break-up model, all other breakup models show a good correlation with experimental observations. Due to lower break-up rates by the PE model, the liquid penetration length is significantly over predicted.

In order to study the effect of atomization models on the mixing field, the radial mixture fraction profiles for different atomization models with the RD break-up model are compared with experimental data at axial distances of 25 mm and 45 mm from the injection location (Figure 3.5(left) and Figure 3.5(right)). The predictions from the RD atomization model are in better agreement with experimental data at both axial locations, while the MPI models show a slight over prediction at 25 mm and large under prediction at 45 mm. This can be explained by a comparison of the centerline mixture fraction (left) and velocity (right) for
Figure 3.7: Temporal evolution of spray penetration and liquid penetration length for the best chosen settings: 0.25 mm, 1 µs, $k - \epsilon$ high Re and RD-RD models, for Spray H (left) and Spray A (right).

three atomization models (Figure 3.6). It is evident that the MPI models predict a higher vapor concentration close to the nozzle exit due to higher evaporation rates cause by the higher relative velocity. And, the vapor penetration at the tip of the spray decreases. This observation corroborates the spray penetration length observations shown earlier (Figure 3.4). Due to the better performance of the RD atomization model in predicting the mixture fraction fields and spray penetration length, it is selected in combination with the RD droplet break-up model in the remainder of the study.

To summarize, the standard $k - \epsilon$ (high Re) model is the chosen turbulence model for its robustness in predicting vapor penetration and is rather insensitive to time step and grid size. A 0.25 mm cell width is selected due to improved prediction of mixture-fraction fields even though the liquid penetration lengths are slightly over predicted. A fine time step of 1 µs is used to accommodate reacting spray simulations. The atomization model has a major impact on spray penetration but shows only a minor effect on the liquid penetration length. As the RD-RD model combination for atomization and droplet break-up gives a superior prediction for the mixing field it will be the default combination for the remainder of the study. The final results for Spray H and Spray A non-reacting cases are shown in Figure 3.7. These model settings in the CFD solver are kept fixed for the reacting spray modeling, which is the main focus of the next sections.

### 3.3 Reacting spray modeling

The general methodology of FGM, applied to model reacting flows, is presented in Section 2.3 of Chapter 2. Here, it is revisited briefly with more pertinent details for applying the method to ECN reacting spray cases. The main method consists of two major parts: one is pre-tabulation of detailed chemistry (i.e. generating the manifold) and the other is coupling this database (as a look-up table) with turbulent flow calculations in the CFD solver. The interaction is depicted in Figure 3.8. The look-up variables and their variances are additional
Scalars which are solved with corresponding transport equations in STAR-CD simulations, next to Navier-stokes equations. The ambient pressure and temperature conditions and the fuel injector configuration details in STAR-CD are varied for the respective cases from the ECN database. The best model settings for turbulent flow and spray formation which are obtained in Section 3.2.2 are applied. The source term due to droplet evaporation in STAR-CD acts as a source to the equations for mixture fraction and its variance. Note that the direct influence of the droplet evaporation on flame structure is neglected since, in these spray applications, all droplets are evaporated well before the ignition location. The source terms of the progress variable, of their variance, including temperature are retrieved from the database using the lookup variables (which are transported in the CFD solver) at each time step.

Figure 3.8: Interaction of CFD-FGM in STAR-CD.

In the preprocessing of 2D tables (shown in Figure 3.8), two different canonical configurations are used independently to generate tables, namely Igniting Counterflow Diffusion Flames (ICDF) and Homogeneous Reactors (HR). The detailed description of both systems is presented in Section 2.3.1 of Chapter 2. The main difference between the two systems is that ICDF takes flow straining on the chemistry into account so it considers the effect of diffusion and transport phenomenon during reactions, while the HR system does not. The ambient conditions, gas and fuel composition serve as the initial and boundary conditions for these systems to generate the table data specific for each case.

In the ICDF method, igniting flames are obtained by solving governing equations starting from an adiabatic mixing frozen state solution at a single strain rate. Here, the strain rate is defined as the partial derivative of the flow velocity in the normal direction to the flow, in a counter flow setup. For these specific (ECN cases) conditions, a value of 500 s\(^{-1}\) is chosen for the applied strain rate as it captures the strain rate dependency on ignition predictability, which is explained in one of the following sections. These igniting flame solutions are tracked in time to capture the auto-ignition process until a steady state is reached. The composition space 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 solu-
tions approach towards the chemical equilibrium state. The detailed chemistry solutions (of igniting and stationary flames) are tabulated as a function of two control variables i.e. mixture fraction ($Z$) and progress variable ($Y$) as described in Section 2.3.2 of Chapter 2. The mixture fraction ($Z$) is defined based on Bilger’s definition. The progress variable ($Y$) 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 ($Y_i$) of carbon dioxide ($CO_2$), carbon monoxide ($CO$) and hydroperoxyl ($HO_2$) are chosen:

$$Y = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{HO_2}}{M_{HO_2}},$$

Equation (3.2)

$HO_2$ is believed to play an important role in the early ignition phase (low temperature combustion), whereas $CO$ and $CO_2$ capture the intermediate and final stage, respectively. Then, the 2D laminar tables are constructed using the above ICDF chemistry data, based on the two control variables. It is also important to note here that the progress variable values will be scaled between 0 and 1 so as to enforce the statistical independence of $Z$ and $Y$.

In the HR system, a 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. The solutions in time domain are transformed into progress variable, and 2D tables are generated. Figure 3.9 is an illustration of the typical solution used for the generation of the ICDF, and the HR database along with the adiabatic mixing line.

The effect of turbulence on chemistry (i.e. the Turbulence chemistry interaction (TCI)) is taken into account by a presumed PDF approach [Peters, 2000] as described in Section

Figure 3.9: Illustration of temperature as a function of mixture fraction for ICDF, HR, and mixing line.
2.3.3 in Chapter 2  The quantities in the 2D table are integrated with a $\beta$-PDF which 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,

$$\tilde{f}(\tilde{Z}, \tilde{Z}^\prime, \tilde{\mathcal{Y}}, \tilde{\mathcal{Y}}^\prime) = \int_0^1 \int_0^1 f(Z, \mathcal{Y}) P(Z \| \tilde{Z}, \tilde{Z}^\prime) P(\mathcal{Y} \| \tilde{\mathcal{Y}}, \tilde{\mathcal{Y}}^\prime) dZ d\mathcal{Y}, \quad (3.3)$$

After $\beta$-PDF integration, a 4D table is obtained. More details about the implementation of the $\beta$-PDF integration can be found in [Kempf et al., 2000, Bekdemir, 2012].

3.4 Results: FGM method enhancements

To validate and improve the capability of the FGM methodology in the current case studies, the following studies are carried out in a systematic way and the results are presented in this section.

1. A-priori study of the FGM method
2. FGM table resolution studies (without TCI) for reacting sprays
3. Effect of TCI for reacting sprays

3.4.1 A-priori study of the FGM method

The main aim of this study is to validate the FGM method in a laminar 1D simulation, prior to its implementation in 3D CFD simulations. This is performed by comparing the solutions from detailed chemistry based CHEM1D simulations (referred to as CHEM1D-Detailed) and laminar FGM table based CHEM1D simulations (referred to as CHEM1D-FGM). Here, the laminar FGM table is generated using the Igniting Counter flow Diffusion Flame (ICDF) approach and the flamelets are obtained from CHEM1D-Detailed simulations. In CHEM1D-FGM, two governing equations for mixture fraction ($Z$) and progress variable ($\mathcal{Y}$) are solved in 1D space instead of solving for all species (generally ranging from 100 to 2000). The source term of $\mathcal{Y}$, and other desired thermo-chemical quantities are interpolated from the laminar FGM tables. The operating conditions of the Spray H baseline case from the ECN database are used as the boundary conditions for these simulations. The conditions of baseline Spray H case are shown in Table 3.2, except that the $O_2$ mole fraction is now 21% since it is a reacting case. For $n$-heptane oxidation chemistry, the detailed reaction mechanism of Andrae [Andrae, 2008] consisting of 633 reactions with 137 species is used.

Firstly, it is intended to assess the sensitivity of the resolution of the laminar FGM table on its performance with respect to the prediction of the ignition delay. So, 2D FGM tables are constructed with different resolutions in $Z$ and $\mathcal{Y}$ space, using the above ICDF solutions with a fixed strain rate $a = 500 \text{s}^{-1}$. These tables are used in CHEM1D-FGM simulations and compared to CHEM1D-Detailed simulations. The studied resolutions are 101x101, 251x251 and 251x501 points in $Z \times \mathcal{Y}$ space, respectively. The grid is uniform.
in \( Z \) direction whilst both uniform and quadratic spacing are used in \( Y \) direction. The quadratic spacing is defined as \( Y_i = Y_1 + \left( \frac{(i - 1)(N_p - 1)}{N_p - 1} \right)^2 (Y_{N_p} - Y_1) \) where \( N_p \) is the total number of points, leading to a much finer spacing at the lower end of the progress variable, i.e. the early phases of ignition. The linear interpolation scheme is still used for all cases. Figure 3.10 shows the rise in maximum temperature of igniting flames (i.e. max \( T(Z) \)) with respect to time, for all CHEM1D simulations. As one can expect, tables with finer resolution show better ignition delay predictability. However the table with quadratic spacing in \( Y \) direction gives the best result with even less points than the best result using a uniform spacing.

![Figure 3.10: Comparison of FGM chemistry with detailed chemistry with different resolution of FGM tables at \( a = 500 \text{ s}^{-1} \).](image)

For the uniform spacing, even increasing the number of points to 501 in \( Y \) direction is not sufficient to match the detailed chemistry solution sufficiently. Hence, a quadratic spacing refined at the early stages is more advantageous (and thus recommended) than increasing the number of points in an equally spaced distribution in \( Y \) direction.

Secondly, the strain rate dependence on ignition delay is compared between FGM chemistry (CHEM1D-FGM) and the detailed chemistry (CHEM1D-Detailed) for the laminar igniting flames. Note that for CHEM1D-FGM simulations, the table generated at a single strain rate i.e. \( a = 500 \text{ s}^{-1} \) is used. The recommended table resolution (101 equi-spacing for \( Z \), and 101 quadratic spacing for \( Y \)) is applied. The 1D simulations for both CHEM1D-Detailed and CHEM1D-FGM are performed for the same boundary conditions (\( T_{\text{ox}}=1000 \text{ K}, T_{\text{fuel}} =373 \text{ K}, p = 4 \text{ MPa} \)) but at varying strain rate. The auto-ignition delay results from this set of simulations are compared, in Figure 3.11 Here, the ignition delay is defined as the time it takes to reach a temperature equal to a 10% rise from its initial value. As expected, the ignition delay becomes longer when the strain rate increases. This holds for the FGM based as well as the detailed chemistry simulations. Until \( a = 1000 \text{ s}^{-1} \)
Table 3.3: Comparison of sensitivity of strain rate on auto-ignition time for detailed and FGM at single strain rate, $a = 500 \text{ s}^{-1}$.

<table>
<thead>
<tr>
<th>Strain Rate ($s^{-1}$)</th>
<th>100</th>
<th>500</th>
<th>1000</th>
<th>1500</th>
<th>2000</th>
<th>2500</th>
<th>3000</th>
<th>3250</th>
<th>3500</th>
<th>3650</th>
<th>4000</th>
<th>5000</th>
<th>5250</th>
</tr>
</thead>
<tbody>
<tr>
<td>Detailed chemistry</td>
<td>0.33</td>
<td>0.38</td>
<td>0.45</td>
<td>0.52</td>
<td>0.59</td>
<td>0.69</td>
<td>0.86</td>
<td>1.01</td>
<td>1.34</td>
<td>2.15</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>FGM at $a = 500 s^{-1}$</td>
<td>0.36</td>
<td>0.39</td>
<td>0.42</td>
<td>0.46</td>
<td>0.49</td>
<td>0.53</td>
<td>0.58</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.71</td>
<td>1.01</td>
<td>1.24</td>
</tr>
</tbody>
</table>

$s^{-1}$, the ignition delay is showing only a minor dependence on a change in strain rate. It is also shown that the predictions from CHEM1D-FGM are comparable to that from the CHEM1D-detailed (see Table 3.3). At higher strain rates (especially near to the ignition limit), a deviation starts to occur but qualitatively the ignition limit is recovered. This behavior confirms that the followed approach with igniting flames at a single strain rate is able to capture the main effect of straining on ignition delay. Apparently the functional dependence of ignition delay with respect to strain rate for laminar flames is captured, especially at lower strain rate cases. As indicated by Bekdemir [Bekdemir, 2012], a possible way to improve this is introducing one extra progress variable.

![Figure 3.11: Strain rate dependence on auto-ignition delay for detailed and FGM chemistry (using a table generated at a single strain rate, $a = 500 \text{ s}^{-1}$), at $T_{ox} = 1000 \text{ K}$, $T_{fuel} = 373 \text{ K}$, $p = 4 \text{ MPa}$.]
3.4.2 FGM table resolution studies (without TCI) for reacting sprays

Next, the FGM method validation and table resolution study is carried out for the full 3D CFD environment to test if the findings in the laminar case can be confirmed in the 3D CFD simulations. The reacting spray simulations are performed with the STAR-CD solver. The best CFD model settings obtained from spray model analysis are used. The Spray H reacting cases from ECN with a complete sweep of ambient $O_2$ concentrations i.e. 21%, 15%, 12%, 10% and 8% are selected for CFD model implementation and validations. The other common Spray H conditions are as shown in Table 3.2.

Here, no TCI model is implemented, or alternatively it can be considered to be a pdf method applying a $\delta$- function (for both control variables) which is also known as a ‘well-mixed’ type of approximation. A few 2D FGM table resolutions (based on an a-priori study) are selected and studied for their sensitivity on the obtained solution. They are 251x251(uniform), 251x501(uniform), 251x501(quadratic), 101x101(quadratic) in $Z$ and $Y$ directions, respectively. The tables are generated using both the HR as well as the ICDF approaches. The results are compared with experimental data and also with a reference simulation case to evaluate the impact of the table resolution on the results. This reference case is based on the first study that applied FGM for such as system [Rijk, 2009]. There a 4D FGM table with coarse resolution (21, 15, 21, 15 uniform grid points in $\tilde{Z}$, $\tilde{Z}'^2$, $\tilde{Y}$, $\tilde{Y}'^2$ and directions respectively) was applied, so note here that TCI was included for this reference case.

The ignition delay predictions from the simulations are compared with measured data. It is to be noted that the measured values of ignition delay are defined based on pressure rise in the combustion vessel. Since the complete vessel is not considered in the current model (see Section 3.2.1), the computed pressure rise will be different from that of the experiments. Hence, using the same definition is not appropriate. Therefore the definition suggested in ECN1 meeting [ECN, 2012] is applied. The ignition delay is now defined as the moment when the temperature of any cell in the domain reaches the value,

$$T_{ign} = T_{in} + \frac{T_{\text{max[converged]}} - T_{in}}{2}, \quad (3.4)$$

where $T_{\text{max[converged]}}$ is the converged maximum temperature in the domain, and $T_{in}$ is the initial temperature (1000 K).

The results are presented in Figure 3.12. It can be found primarily that the FGM method captures the ignition sensitivity with respect to the $O_2$ change, qualitatively even with the coarse table resolution, for both ICDF and HR tabulation approaches. However, the quantitative trend is improved dramatically by implementing finer table resolutions. Noticeably, there is still a difference between uniform and quadratic cases at finer resolutions, and similar to the a-priori analysis, the ignition delay times are comparable for both quadratic cases with different table resolution sizes (shown in black and green). These observations are independent of the used generation method (HR or ICDF). So, from this comprehensive 3D CFD study and the 1D a-priori studies, it is revealed that applying a quadratic spacing in
the grid in $Y$ direction with 101 points (in both directions) is adequate to achieve sufficient accuracy for the ignition delay predictions.

Figure 3.12: The effect of table’s resolution on ignition delay for ICDF (left) and HR (right) approaches.

Figure 3.13: The ignition delay predictions from ICDF (green) and HR (red) approaches compared against experimental data from ECN database (blue).

The best results are plotted in Figure 3.13, for both generation approaches. The model predictions are slightly under-predicted (10-25%) compared to the experimental values, however the trend is very well captured. Another interesting observation is that tables generated using HR and ICDF approaches predict similar ignition delay timings, which is not
expected. This might be due to the fact that for this operating condition (with elevated ambient temperature i.e., 1000 K), straining does not play a significant role during the ignition process. In order to investigate this outcome further, the data from both tabulation methods are compared, for one chosen case ([O$_2$]=15%). In Figure 3.14, the temporal evolution of the average source term of $\mathcal{Y}$ from CFD simulations is plotted. The magnitudes of these quantities are small (when compared to the values of tabulated source term itself, see Figure 3.16) due to the averaging over the entire computational domain. The model with HR based FGM picks up higher source terms than the model with ICDF based tables as expected. Nevertheless the early rise of the source terms occurs at the same time which is important to predict ignition delay and has a similar shape (see red circle). Only in the second phase a difference occurs.

![Figure 3.14](image.png)

**Figure 3.14**: Time evolution of average source $\mathcal{Y}$ from CFD simulations with ICDF based FGM (green) and HR based FGM (red), for [O$_2$]=15% case.

The scatter data for progress variable against mixture fraction at three time instances just before the ignition is compared from two simulations with the two different FGM tabulations, in Figure 3.15. This shows a comparable behavior at the time of ignition for both approaches and most importantly the $\mathcal{Y}$ rise occurs mainly around a mixture fraction of 0.1. In order to understand this similarity further, in Figure 3.16, the source terms of $\mathcal{Y}$ from both 2D tables are studied. The HR based FGM table shows higher (one order magnitude) source terms compared that from the ICDF based FGM table, at relative fuel rich zones ($Z=0.25$-0.35). However, the ignition in CFD simulations happens at mixture compositions that are typically leaner than $Z=0.25$ (as observed in Figure 3.15 still richer compared to $Z_{st}$) for these high ambient temperature conditions. At these mixtures (around $Z=0.1$), the source terms of $\mathcal{Y}$ from both tables are quite comparable (same order of magnitude) as shown in Figure 3.16 (bottom), with the marked region. This is especially true at low values of $\mathcal{Y}$
(early stages of ignition). Hence the ignition chemistry path in CFD computations for this condition is not affected significantly using two different FGM tables.

The flame liftoff length (LOL) is another important characteristic that has been studied, in addition to ignition delay. This parameter is used to characterize the flame structure and
generally, it is described as the most upstream location of the stable flame away from the injector hole. According to the ECN group, LOL is defined as the distance between tip of the injector and the cell in the computational domain where the $OH$ mass fraction reaches a threshold value of 0.00025. Although $OH$ chemiluminescence experiments are based on excited $OH$ states ($OH^*$) and not stable $OH$ species, since the reaction mechanisms do not contain the excited $OH^*$ states, the definition based on stable $OH$ species is widely used to calculate the LOL from simulations results. This definition is used for this study.

![Figure 3.17](image)

**Figure 3.17:** The temporal evolution of liftoff length (LOL) from ICDF based FGM simulations. (LOL defined using threshold of $Y_{OH} = 0.00025$).

The typical behavior of the igniting diesel spray is that, after the auto-ignition, the flame propagates upstream and stabilizes at a certain point. Figure 3.17 shows this temporal evolution of liftoff length predictions from the simulations with ICDF based FGM tables for different $O_2$ concentrations. Here, FGM tables with resolution of 251(uniform) in $Z$ and 501(quadratic) in $Y$ are being used. The LOL is calculated as a function of time to determine the settling time, and the corresponding LOL is considered as the final LOL distance. In general, for all $O_2$ concentrations cases the LOL converges after $t = 3ms$. This is also observed for simulations using HR based FGM tables.

Now, in Figure 3.18 (left), all converged LOL results from both tabulation approaches are presented along with experimental data. The LOL sensitivities with respect to $O_2$ change is captured well by the models, qualitatively. However, the magnitudes are differing from the experimental data consistently for both methods. It is to be noted here that quantitative agreement with experimental data is subject to the definition of LOL as it corresponds to a fixed value of $OH$ mass fractions (0.00025) in the resolved igniting flame structure. Figure 3.18 (right) shows the correlation between LOL and ignition delay from both experimental and simulated results. HR based simulations follow the roughly linear trend similar to the experimental values, whereas ICDF based simulations deviate slightly. The 12\% $O_2$ case with the higher deviation (around 20\%) is chosen to investigate the cause for these differences between the two tabulation approaches. Figure 3.19 shows the contours for $Z$, $Y$ and
Figure 3.18: The liftoff length comparison between the FGM method and experiments, as a function of (left) $[O_2]$ and (right) ignition delay.

Figure 3.19: Contours of $Z$ (top), $Y$ (middle) and $OH$ mass fraction (bottom) from CFD simulations with FGM based on ICDF (left) and HR (right), at 3ms for $[O_2] = 12\%$ case.

$OH$ mass fraction (from top to bottom) from the simulation with FGM based on ICDF (left) and HR (right), for 12\% $[O_2]$ case.

Firstly, the flame structures shown by the $Z$ and $Y$ field are different for the two CFD simulations. The mixture fraction field is affected due to the influence of the resolved temperature field on the local evaporation rate of fuel. The differences in $Y$ field is attributed by the fundamental differences in tabulated source terms of $Y$ from two different tabulation databases, at the time of flame stabilization. Secondly, as the $OH$ field is retrieved from the table, the two $OH$ distribution differences in the manifolds will induce differences in
space and time. This can be seen in Figure 3.20, where the $OH$ mass fraction contours as a function of $Z$ and $Y$ from the chemistry databases of ICDF (left) and HR (right) are plotted. Mainly, the ICDF based FGM leads to low $OH$ fields in a wide range of $Z$ and $Y$, whereas the HR based FGM leads to more localized $OH$ fields within a broad range of $Z$ at a narrow range of $Y$. Hence, the $OH$ magnitudes in CFD simulations are considerably affected by the tabulation methods. Importantly, since the stabilization for LOL is defined by very small threshold value of $OH$, the observed differences in Figure 3.20 will have a real impact on LOL predictions.

To summarize, the ignition delay predictions from both tabulation methods are quite similar at these high temperature ambient conditions while the large differences in $OH$ fields from the two tables lead to differences in the prediction of LOL which is defined based on a single threshold value of $OH$. Hence, so far, it can be indicated that both methods are performing comparably similar.

### 3.4.3 Effect of TCI for reacting sprays

Further, the effect of $Z''^2$ (i.e., TCI model) is investigated by including it in FGM tables. The tables are integrated using a presumed pdf functions in $Z$ direction and the 2D tables are converted into 3D tables. Initially, the $Z''^2$ data from CFD is analyzed to determine the adequate number of levels of $Z''^2$ in the FGM table. Figure 3.21 depicts a typical field from the simulation with $[O_2] = 8\%$ with ICDF based FGM at different time steps along with the data from FGM table. Similar fields are found for both methods at different oxygen level cases and at various other time steps. 9 levels of variance of $Z$ are applied along with 101 points in $Z$(uniform) and $Y$(quadratic) directions.

A new set of simulations for different $O_2$ concentration cases are performed with the 3D FGM table. The ignition delay and liftoff length characteristics are processed and plotted in Figure 3.22, for with (black) and without $Z''^2$ (red) for ICDF based FGM (left) and

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**Figure 3.20**: Contours of $OH$ mass fraction (bottom) from ICDF based FGM (left) and HR based FGM (right), for $[O_2] = 12\%$ case.
HR based FGM (right) along with experimental data (blue). The influence of $\bar{Z}''^2$ on ignition delay prediction is not significant, however a slight reduction in ignition delay timing is observed at low $O_2$ cases. Intuitively, this is not expected as the pdf integration leads to lower maximum source terms and was expected to result in longer ignition delay. Hence it is further investigated.

**Figure 3.21**: A typical $Z-Z''^2$ field for $[O_2]=8\%$ in ICDF based FGM simulations. Red dots represent the points in the corresponding FGM table with 9 levels of $Z''^2$.

**Figure 3.22**: The effect of $\bar{Z}''^2$ on ignition delay, liftoff length for ICDF (left) and HR (right) approaches.
In Figure 3.23, the evolution of the source of $\mathcal{Y}$ from ICDF based FGM (top) and HR based FGM (bottom) simulations with (blue) and without $\bar{Z}''^2$ (red) is plotted for 8% case, just before the ignition event. The broken line (black) refers to the stoichiometric mixture fraction (i.e. $Z_{st}$ which is 0.0245 for this case). The introduction of the $\bar{Z}''^2$ results in a broader distribution of the source terms, and lowers the peak values (especially at initial times i.e. 0.9 ms, 1.1 ms). The broader distribution introduces higher source terms at the leaner mixtures and close to $Z_{st}$. Since ignition happens more towards $Z = Z_{st}$, the increase in source terms at these mixtures favors an early ignition for cases with $\bar{Z}''^2$ when compared to without $\bar{Z}''^2$.

It is evident from this analysis that the introduction of $\bar{Z}''^2$ does not necessarily reduce the source terms of progress variable. Especially at early stages, this introduction may result in an increase in chemical source terms, at leaner mixture side where ignition starts. As an example, the effect of $\bar{Z}''^2$ is shown for both ICDF and HR based FGM, at $Z=0.01$ and $\mathcal{Y} = 0.058$ in Figure 3.24(left). In this example, pdf integration increases the source terms for both methods. In Figure 3.24(right), a further illustration at one variance point is given for HR based FGM. According to the mean and variance levels of $Z$, a $\beta$-function is defined for every point in the manifold which is shown in blue curve. The green plot represent the source terms of $\mathcal{Y}$ over the mixture fraction domain at a specific $\mathcal{Y}$ point. Now this quantity is integrated using the pdf function. When one single point (at $Z = 0.3$) is identified, then it is found that the integrated quantity of the source term (red diamond) is higher than the corresponding value at $Z=0.3$ (black triangle).

The effect of the inclusion of $\bar{Z}''^2$ on flame liftoff length is studied now. However,
primarily it should be noted here that the CFD simulations for low \( O_2 \) concentrations did not yield the threshold value of \( OH \) mass fraction (=0.00025) which is typically used as a measure of LOL. It is also reported by many other modeling groups in the ECN community. Hence an alternative definition for LOL is suggested in ECN, which has been used in this part. According to this definition, LOL is defined as the first axial point where the \( OH \) mass fraction reaches 2% of the maximum in the domain after a stable flame is established. From Figure 3.22 it can be seen that the predicted trends of LOL with respect to change in \( O_2 \) is consistently smaller with inclusion of \( \tilde{Z}''^2 \). Both methods show similar trends.

**Figure 3.24:** (left) The effect of \( \tilde{Z}''^2 \) on \( \mathcal{Y} \) source terms of ICDF based FGM table and HR based FGM table, at \( Z=0.01 \) and \( \mathcal{Y}=0.0576 \). (right) Comparison of source term of \( \mathcal{Y} \) before and after pdf integration along with pdf function for HR based FGM table, at \( Z=0.3, \mathcal{Y}=0.1681, \tilde{Z}''^2 = 0.0026 \).

**Figure 3.25:** Temperature (top) and \( OH \) mass fraction (bottom) contours without \( \tilde{Z}''^2 \) (left) and with \( \tilde{Z}''^2 \) (right) for \( O_2=12\% \) case, at \( t=3\,ms \) from ICDF based FGM simulations.
The effect of $\tilde{Z}''$ on temperature and $OH$ mass fraction fields at 3 ms from ICDF based FGM simulations for the 12% $O_2$ case is presented in Figure 3.25. The introduction of $\tilde{Z}''$ reduces the peak values in the flame structure by distributing them to wider regions. The broader distribution of $OH$ leads to a shorter LOL and the flame stabilization location moves closer to the nozzle exit. Hence, the inclusion of $\tilde{Z}''$ results in considerably lower LOL.

It is also observed that the inclusion of $\tilde{Z}''$ improved the model sensitivity for LOL with respect to the change in $O_2$, particularly in case of ICDF based FGM. This is due to the fact that LOL (defined based on $OH$ mass fraction) is more sensitive for low $O_2$ percentages due to the lower $OH$ values. In Figure 3.26 the effect of $\tilde{Z}''$ on the correlation between liftoff length and ignition delay is shown for ICDF and HR based FGM along with experimental data. In case of the ICDF based FGM, the inclusion of $\tilde{Z}''$ improves the LOL match with experiments by capturing the relation between LOL and ignition delay, mainly for the shorter ignition delays. For HR based FGM, deviation from experiments increases particularly at longer ignition delay timings (for lower $O_2$ concentrations) due to the effect of $\tilde{Z}''$.

In a nutshell, the effect of FGM table resolution and TCI model on the predictions is assessed for spray-H reacting cases. It is revealed that a resolution of 101 x 9 x 101(quad) x 1 in $\tilde{Z} x \tilde{Z}'' x \tilde{Y} x \tilde{Y}''$ is adequate to capture ignition delay and liftoff length trends observed for the studied sweep in $O_2$ concentration. Although change in tabulation method do not show significant effect on ignition delay, HR based FGM shows consistently underpredicted LOL against experiments when compared to that of ICDF based FGM. In order to test this further at various operating conditions, the method is applied to an extensive
Table 3.4: Parametric sweep of Spray A reacting conditions.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient Temperature (K)</td>
<td>750, 800, 900, 1100</td>
</tr>
<tr>
<td>$O_2$ concentration [%]</td>
<td>13, 15, 21</td>
</tr>
<tr>
<td>Ambient Density ($kg/m^3$)</td>
<td>7.6, 15.2, 22.8</td>
</tr>
<tr>
<td>Injection Pressure (MPa)</td>
<td>50, 100, 150</td>
</tr>
</tbody>
</table>

parametric study using a different fuel which will be discussed in next section.

3.5 Results: Parametric study

The main purpose of this work is to apply and validate the FGM method for a large set of operating conditions available for the Spray A reacting case from ECN database [ECN, 2012]. The main difference with Spray H is that the fuel used here is $n$-dodecane instead of $n$-heptane. Hence it is an interesting test case to assess the robustness of the FGM method with respect to the fuel used. Moreover, the ambient condition is more representative for a relatively low temperature combustion condition relevant for engines with moderate EGR. The set of operating parameters (in a constant vessel setup) that is considered for this parametric sweep is ambient temperature, $O_2$ concentration, ambient density and injection pressure. These are to mimic the charge temperatures at early injection timings (in new engine combustion concepts), compositions with change in EGR conditions, the charge boost pressure conditions and rail pressures, respectively. Table 3.4 shows the chosen values of these parameters along with the baseline condition (in bold). The other common operating conditions of Spray A can be seen in Table 3.2.

Simulations are performed for these parametric variation cases. At each parametric sweep, the other parameters are kept fixed to the baseline conditions. These parametric changes serve as the boundary conditions to generate corresponding FGM tables. Again ICDF and HR based tabulation approaches are used to obtain two sets of tables at each condition. The ambient temperature and $O_2$ concentration is imposed as oxidizer conditions, and ambient density defines the pressure of the mixture. The change in injection pressure is applied by varying the injection rate in the spray model of STAR-CD solver. The same CFD model settings used in the earlier study are applied. The best FGM table resolution is applied in this study i.e. 101 points in each $Z$ (uniform), $Y$ (quadratic) directions and 9 points in $\tilde{Z}^{\prime\prime}$ direction, respectively. Note that effect of $\tilde{Y}^{\prime\prime}$ is omitted due to it insignificant effect on ignition prediction, hence $\delta$-function is used for $\tilde{Y}^{\prime\prime}$ i.e. one single point in this direction. Since the diesel surrogate fuel used in Spray A is $n$-dodecane which is new to the research community, getting a reaction mechanism is an additional challenge here for modeling purpose. The reaction mechanism from Narayanaswamy and Pitsch [Narayanaswamy et al., 2013], which is one of the very few smaller mechanisms that are under development at present, has been used to generate laminar chemistry in CHEM1D solver. This mecha-
nism consists of 253 species and 1437 reactions including PAH chemistry up to 4 rings. It is worth to note here that the advantage of the FGM method is the efficiency in handling such a huge mechanism.

The typical two ignition characteristics from simulations for all the above cases have been compared with the experimental observations that are obtained by [Benajes et al., 2013], from the ECN database. In order to have a fair comparison, the definition agreed during ECN 2 meeting [ECN, 2012] is used for ignition delay and liftoff length. Again the ignition delay time is defined as the time at which the maximum rate of rise of maximum temperature achieved in the domain and the liftoff length location is defined as the first axial location of $OH$ mass fraction reaching 2% of its maximum in the domain. Typically this length evolves with time. Therefore the final stabilized location is treated as the liftoff length (see Figure 3.17).

*Figure 3.27: FGM Model sensitivities on ignition characteristics with parametric sweep of Ambient Temperature (left) and $O_2$ concentrations (right) compared with experimental data (in blue). The two tabulation approaches are shown: ICDF (in green) and HR (in red). In order to visualize the sensitivity, different scales are used. $\rho = 22.8$ kg/m$^3$, Rail Pressure = 150 MPa.*

In Figure 3.27, ignition delay and liftoff length (LOL) sensitivities with respect to change in ambient temperature (left) and ambient $O_2$ concentration (right) have been plotted, respectively. Both models predict the ignition delay trend for the complete $O_2$ concentration change (at $T = 900$ K) with a good agreement against the experimental data. Quantitatively, ICDF based FGM is slightly over predicting (5-20%) whereas HR based FGM is under predicting (30-35%) when compared to experiments. On the other hand, both models predict the increasing trend of ignition delay time with decrease in the ambient temperature (at $[O_2] = 15\%$). The approach with HR based FGM shows a very good agreement with experimental data throughout the temperature variation whereas the model with ICDF based FGM shows an over-predicted sensitivity when moving towards the relatively lower temperatures i.e. 800 K and beyond. Especially at 750 K, the ICDF based FGM model over predicts the ignition delay by two times. This must be due to the effect of flow staining on the chemistry which is the only main difference between these two tabulation approaches as described in Section 2.3.1 of Chapter 2. So, in order to investigate this further, the flow
straining effect is studied.

Firstly, the typical range of the straining that the flow field imposes in this kind of CFD simulations is determined in terms of the strain rate, which is the parameter used to compute the igniting flames in CHEM1D. For that purpose, the scalar dissipation rates from the CFD model and igniting flames at different strain rates are compared as shown in Figure 3.28.

**Figure 3.28:** (Left) scatter plot of scalar dissipation rate vs. mixture fraction, from CFD modeled data at two simulations times, and pdf integrated data from igniting flames at different strain rates (at oxidizer side, \( a = \frac{(du_y)}{dy} \)). (Right) The zoomed view shown by the dotted box for better illustration.

The turbulent mean value of scalar dissipation rates from CFD (using equation 3.5) are plotted against mixture fraction, at two different time instances.

\[
\tilde{\chi} = c_\chi \frac{\tilde{\epsilon}}{\tilde{k}} Z''^2, \tag{3.5}
\]

where \( \epsilon \) is eddy dissipation rate and \( k \) is turbulent kinetic energy, \( c_\chi \) is coefficient (=2.0). Similarly, the mean scalar dissipation rate of the ICDF's, \( \tilde{\chi}(Z, Y) \), according to,

\[
\tilde{\chi}(\tilde{Z}, \tilde{Z''}^2, \tilde{Y}, \tilde{Y''}^2) = \int_0^1 \int_0^1 \chi(Z, Y) P(Z \parallel \tilde{Z}, \tilde{Z''}^2) P(Y \parallel \tilde{Y}, \tilde{Y''}^2) dZdY, \tag{3.6}
\]

are determined for several strain rates. Here, \( \chi(Z, Y) = 2D_z \left( \frac{\partial Z}{\partial X} \right)^2 \bigg|_a \), with \( D_z \) - the diffusion coefficient for \( Z \). Due to the integration of \( \chi \) in both control variables and their variances, the resulted average data has a wide spread as shown in Figure 3.28 From the comparison (Figure 3.28), it is found that scalar dissipation rate encountered by flow straining is enclosed by scalar dissipation rate from the ICDF’s with applied strain rates up to 2500 s\(^{-1}\).
Figure 3.29: The auto-ignition delay (from detailed chemistry simulations) as a function of applied strain rate in CHEM1D for ICDF, at different ambient temperatures (top) and $O_2$ concentrations (bottom). Range of straining exerted in CFD flow is marked in red dotted box.

The effects on ignition of the ICDF for these strain rates have been studied in detail. In Figure 3.29, the strain rate dependence on ignition delay time is plotted for different operating conditions, for the ambient temperature sweep (top plot) and ambient $O_2$ concentrations (bottom plot). The range of strain rates associated with the CFD flow field is marked (in broken red lined box) in the figure. It is clear from this plot that the detailed chemistry is rather sensitive to the straining exerted in the flow field at low temperature conditions like 800 K and 750 K. Now, the overestimation by the ICDF based FGM model might associated to the fact that the single strain rate ($i.e.$, $500 \text{ s}^{-1}$) used while generating igniting chemistry flamelets for the FGM table is close to the ignition limit for these low temperatures conditions.

To test this, two more ICDF tables are generated at 800 K condition using igniting flamelets at lower strain rates $i.e.$, $100 \text{ s}^{-1}$, $2 \text{ s}^{-1}$ (instead of conventional value of $500 \text{ s}^{-1}$) and are coupled to the CFD simulations. The results are presented in the Figure 3.30 in combination with the results from ICDF based FGM (at 500 $\text{s}^{-1}$) and the HR based FGM model. When compared to the predictions of FGM based on ICDF (at $500 \text{ s}^{-1}$), the predictions of the FGM based on ICDF (at lower strain rate) are improved by lowering the ignition delay time, which is an expected trend with lower strain rates. However, the location of liftoff length deviates more from the experimental value and moves towards the injector hole. This shows that the ICDF based FGM with low strain rate behaves similar to the HR based FGM, where the chemistry by definition is not affected by the flow straining.
Figure 3.30: FGM model predictions for ignition delay (Left) and liftoff length (Right) with ICDF at three different strain rates, and with HR, compared with experimental results for the case: 800 K, 15% \[O_2\], 22.8 kg/m^3 and 150 MPa injection pressure.

(i.e. \(\chi = 0\)), as expected.

Figure 3.31: Schematic of typical Negative Temperature Coefficient (NTC) behavior of \(n\)-alkanes [Bouali et al., 2012].

The deviation of ICDF based FGM’s predictability at low temperature conditions is mainly attributable to two reasons. First; at these conditions the flow induced straining is closer to the ignition limit and the set of lookup variables to capture the effect near to the ignition limit is not sufficient. This is also consistent with the conclusions from FGM - DNS based studies in [Bekdemir, 2012]. There, it was suggested to extend the manifold with an extra variable i.e., mass fraction of \(HO_2\) which showed a monotonic dependency on strain around the ignition region. Second; as known from the shock tube, pressurize flow reactor studies detailed reaction mechanism typically have a problem capturing ignition delay
at low or intermediate temperatures [Westbrook et al., 2009; Narayanaswamy et al., 2013] which are known as Negative Temperature Coefficient (NTC) zone. The ignition delay in this zone is mainly determined by the competition between high and low temperature reactions. Figure 3.31 depicts the schematic of typical NTC zone where the ignition delay changes its course due to the transition from low temperature to high temperature regions. So even if the FGM table would be extended the experimentally observed ignition delay might not be recovered.

![Figure 3.31: Schematic of typical NTC zone.](image)

Figure 3.32: Contours of OH mass fraction (bottom) from the tables, ICDF based FGM (left) and HR based FGM (right), for baseline Spray A case.

Similarly, the predicted liftoff lengths by the ICDF based model follow the experimental trend till 800 K as shown in Figure 3.27(left). However, at 750 K the quasi steady state of the flame is never achieved and moves downstream till the end of the simulation (similar case with HR based model). Hence, the LOL results for the 750 K case are not provided in the plot. The LOL of HR based model is insensitive to the change in ambient temperature conditions. For the sweep of $O_2$ concentrations, as shown in Figure 3.27(right), ICDF based model captures the liftoff length sensitivities accurately compared with experiments, whereas HR based model is completely insensitive. This stems from the main fact that the two tabulation methods lead to different distributions and levels of OH in FGM tables (as shown in Figure 3.32) which effects the stabilization location significantly.

In Figure 3.33, the model sensitivities with respect to change in ambient density (left) and injection pressure (right) have been presented along with the experimental data. The predictions from ICDF based FGM show a very good agreement to experimental observations for both ignition delay time and liftoff length location. The minor deviations observed in terms of magnitudes can be pertained to the definitions of LOL that are agreed upon and the potential improvements expected through the incorporation of the straining dependency in the FGM table using an extra control variable. The HR based FGM also shows a similar trend compared to the experimental observations. However it shows a lower sensitivity to the changes in the ambient density.

In Figure 3.33 (right), the effect of a change in injection rail pressure on ignition delay and liftoff length are compared between models with ICDF and HR against the experiments. During the modeling setup, only the injection flow rate is varied to account for the change
in injection pressures while the same FGM tables are being used in the simulations. Hence, the only two factors that can contribute to the accuracy of model predictions are (1) the ability of the spray models to capture the change in spray (mixture) formation, and (2) the response of the FGM model with tabulated chemistry to such changes in the flow field. According to experimental data, an increase in injection pressure decreases the ignition delay and increases the liftoff length. ICDF based FGM model captures the influence on ignition timing and flame liftoff length associated with the change in flow field due to the change in injection pressures. However the HR based FGM is relatively insensitive to the changes in injection pressure. The contours from the CFD simulations are studied to further investigate these differences.

**Figure 3.34**: $Z$ (left) and $OH$ mass fraction (right) contours for injection pressure of 50 MPa (top) and 150 MPa (bottom) case, at $t = 3$ ms from ICDF based FGM simulations.

In Figure 3.34 and Figure 3.35 the contours from CFD simulations for ICDF based FGM and HR based FGM are shown respectively. The $Z$ (left) and $OH$ mass fractions (right) are compared for two different injection rail pressure conditions (50MPa (top) and 150MPa (bottom)). It is clear from the $Z$ fields that the increase in injection pressure leads
to larger penetration lengths. The $OH$ fields from ICDF based FGM simulations show a steep rise locally with increase in injection pressure and eventually the flame stabilization point moves away from the injector hole. In case of HR based FGM simulations, with increase in injection pressure, the rise in $OH$ fields is gradual and wide spread, leaving the flame stabilization point relatively unchanged and close to the injector hole. This stems from the fact that the $OH$ fields in FGM tables of an ICDF is more localized in $Z$ space while it is more widely distributed in the HR based tables, as shown in Figure 3.32. However, it is important to note here that the flame structures shown by two tabulation methods are comparable. The used definition of stabilization locations is the source for the effect that is seen in the LOL results. This in fact points to the main shortcoming of the current dataset which is mostly based on global measures like ignition delay and LOL. The experimental database needs to be extended to include field data of species like $OH$, and temperatures which are currently pursued by the research groups. Global measures are not sufficient to make a well balanced judgment on the adequacy of the numerical methods as is also argued by others e.g. [Bhattacharjee and Haworth, 2013].

### 3.6 Conclusions

The FGM method is applied to model dedicated single igniting diesel spray characteristics in a constant volume combustion vessel. To set up the flow and spray formation, Lagrangian two phase spray models are used with RANS based simulations in STAR-CD. The sensitivity of these model settings such as cell size, solver time step, turbulence models and the spray sub models on non-reacting spray characteristics (namely liquid and spray penetration lengths) and mixture fraction profiles is assessed. The best combination is selected based on satisfactory agreement with the experimental data for Spray H ($n$-heptane) and Spray A ($n$-dodecane) non-reacting conditions from the ECN database. Further, these model settings are fixed during the subsequent reacting spray modeling studies. The FGM tables generated using detailed chemistry are coupled to the CFD solver to model the turbulent reacting spray along with the auto-ignition phenomenon. In the current research study, two different generation techniques (ICDF and HR) are used to investigate the role of the transport and diffusion process on the chemistry tabulation and its effect on the predictability of ignition. The first important feature of the FGM table which can affect the results is the chosen resolution in both the dimensions i.e. $Z$, $Y$. The a-priori study based on 1D counterflow flames
in CHEM1D revealed that the FGM based chemistry can reproduce the detailed chemistry accurately with finer table resolutions, and more importantly the quadratic spacing in direction is vital. Using that including 101 points in each direction is adequate. Further, a laminar table’s resolution study is carried out in 3D CFD model for a wide range of $O_2$ concentrations of Spray H conditions. The results reinforce that the finer table resolution (i.e. 101 points in each direction) with quadratic spacing in $Y$ direction improves the predicted trends for the ignition delay, for both tabulation approaches. The results also validate the FGM model’s ability to predict the ignition delay accurately. For this applied condition (with high ambient temperature and shorter ignition delay), the two different tabulation approaches predict similar ignition timings due to the fact that the significance of transport and diffusion on the ignition process is low. Flow straining is well away from the strain induced ignition limit. Moreover the differences in $OH$ fields of these two methods resulted in different flame stabilization locations and eventually shorter liftoff length (which is based on $OH$ mass fraction) for the method where HR’s were used. However, the model predictions are qualitatively in good agreement with the experimental trends of LOL vs. $O_2$ sweep. Subsequently, the FGM tables are extended with $Z$ variance ($\tilde{Z}''^2$) to study the turbulence chemistry interaction on ignition process. The inclusion of $\tilde{Z}''^2$ shows negligible effect on ignition delay timing, whereas it reduces the LOL values. The latter is due to the fact that including TCI leads to a broader distribution of $OH$ mass fractions. Consequently (due to its definition) the LOL appears to move towards the nozzle. However, to our opinion this points more towards the hampered definition of the LOL (2.5% of the max $OH$) compared to its experimental value (based on $OH^*$ emissions).

The enhanced FGM model with best table resolution and TCI is applied to various parametric sweeps available for Spray A to validate the model sensitivities against the experimental observations from the ECN database. The model with ICDF based FGM captures the sensitivities for both the ignition delay timing and LOL with change in the ambient temperature, $O_2$, ambient density and injection pressure well. At low temperatures, where the ignition is highly sensitive to flow straining, the method over-predicts ignition timings and flame structure is altered. The predictions might be improved if the FGM method is extended with another dimension to control the straining influence more directly. On the other hand, the HR based FGM model captures the trends of ignition delay with change in conditions even at low temperature conditions, whereas it is unable to capture the LOL sensitivity. Again the major source for these differences in LOL predictions is probably caused by the chosen definition based on $OH$ fields, and the contribution by the differences in $OH$ fields. Availability of measurement data for more species may lead to better and reliable LOL analysis.

Finally, it is concluded that the FGM model with adequate settings with respect to table resolution and TCI shows good ignition characteristics i.e. ignition delay timings and flame liftoff location for various engine relevant conditions. It is able to capture changes in fuel, ambient conditions and injection pressures. Hence, the model is applied for engine cycle simulation in the further studies which are presented in next chapter.
FGM approach for Engine Cycle Simulations

Most of the work is carried out by the author himself, while the model implementation for PCCI case is done by his colleague U. Egüz. The content is extracted from the following publications, and minor additions/changes are made to improve the quality and structure of the chapter.


4.1 Introduction

Diesel spray combustion in engines consists of a complex two phase flow in combination with a combustion event involving a vast amount of species and reactions in a time varying geometry. Modeling such an event is highly challenging not only due to its inherent complexity but also due to its sensitivity to the changes in the operating conditions such as injection timing, Exhaust Gas Recirculation (EGR) levels, etc. On the other hand, given the current complexity of engines, experiments are expensive, time consuming and have limited accessibility. Hence, a robust combustion model setup could help to assess such varying diesel combustion phenomena but it calls for a continuous improvement of existing models to make them more dependable and predictive.

There are several combustion modeling approaches found in literature which are ranging from mixing models such as the eddy dissipation model [Magnussen and Hjertager, 1977], mixing/characteristic timescale models [Abraham et al., 1985, Patterson et al., 1994, Kong et al., 1995] and Flamelet models. The latter which encompass a large spectrum such as the Coherent Flamelet model [Martinot et al., 2001], Flamelet time scale model [Hu and Rutland, 2006, Hu et al., 2008], Representative Interactive Flamelet (RIF) model [Pitsch et al., 1996, Singh et al., 2006], Transient Interactive Flamelet (TIF) model [Lehtiniemi et al., 2008] and Transient Flamelet Progress Variable (TFPV) model [Lehtiniemi et al.,
One of the main output interests of modeling is predictions of pollutant emissions which are dependent on local species distribution and temperature. Hence the inclusion of detailed chemistry is indispensable. Although these flamelet methods have many advantages, they still suffer from limitations to apply them in various combustion regimes. Some of them still are computationally expensive, and complex to implement. However, the chemistry tabulation based methods offer an attractive solution with better computational efficiency. The Flamelet Generated Manifold (FGM) methodology is one of such computationally efficient chemistry tabulation methods where the entire detailed chemistry is included using the same conceptual framework as the ‘flamelet’ theory [Peters, 1984], but applying the ‘parametrization’ philosophy of ILDM [Maas and Pope, 1992]. From various studies, FGM has proven to be a robust model for modeling turbulent combustion in many different applications [van Oijen and de Goey, 2004 Vreman et al., 2008 Bongers, 2005]. Recently, the approach is extended to model diesel spray ignition characteristics, using the STAR-CD model framework. In the context of the Engine Combustion Network (ECN) [ECN, 2012], it was extensively validated against experimental data for Spray H, Spray A with n-heptane, n-dodecane as surrogate fuels, respectively. The enhanced model shows a very good agreement with experimental observations on the ignition delay and flame liftoff length. These studies, which are discussed in Chapter 3, build confidence on the application of the FGM methodology for diesel spray combustion modeling.

In the past, the first implementation of FGM tables generated at a single average pressure (and oxidizer temperature) condition in engine cycle simulations [Bekdemir et al., 2009] showed promising directions. Later, the model is improved by pressure dependent FGM in order to study the improvements in the ignition predictability [Bekdemir et al., 2011]. These studies have been performed only at conventional injection timing. Some of the major recommendations from these studies were to apply a more detailed n-heptane mechanism, implement a finer FGM table resolution and incorporating a heat loss model.

In the present work, firstly an improved model with better treatment of the evaporative fuel scalar is implemented for engine cycle simulations, and the improvements are studied (see Appendix A). The best FGM table resolution and more detailed n-heptane reaction mechanism that resulted from an extensive study on the ignition characteristics of Spray H from ECN, given in Chapter 3, is used. Subsequently, the pressure dependent FGM model with the above enhanced model settings is applied to early (Premixed Charge Compression Ignition regime: PCCI) and conventional injection (Classical Diesel Combustion regime: CDC) timings. Typically, the combustion in PCCI conditions (locally) takes place under a well premixed condition or nearly homogeneous mixture of fuel and oxidizer. Hence in this study, a Homogenous Reactor (HR) based FGM database is created for the PCCI case (since the ignition is primarily dictated by reaction kinetics) whereas Igniting Counterflow Diffusion Flames (ICDF) flames are used for the CDC database applied for conventional cases as it characterizes predominantly diffusion like flame structures. The main objective of this study is to evaluate the improvements in model predictions due to these model enhancements for the CDC case and to investigate the model ability to predict ignition while extending it to early injection conditions like PCCI [Ayyapureddi et al., 2013]. Eventually, the FGM model is extended with enthalpy as an additional dimension besides mixture fraction, its variance, progress variable, and pressure in order to account for the heat loss effect during engine cycle simulations. Finally, Nitrogen oxide formation ($NO_x$), which is highly
temperature dependent, is modeled in order to study the effect of model enhancements for the CDC case.

The outline of this chapter is as follows: First, the modeling framework is presented with a short overview followed by a more detailed description of each aspect of the modeling approach. Then, the details of model setup, engine data for the chosen operating conditions are provided. In subsequent sections, the pressure dependent FGM with improved model set up is applied to CDC and PCCI conditions and the results for combustion characteristics are presented. Next, an a-priori study is carried out to extract the enthalpy levels needed for implementation of the enthalpy dependent FGM model. Then eventually, the $NO_x$ model implementation is described and results are presented with the improvements due to model enhancements i.e. accounting for the heat loss effect. Finally, conclusions are discussed and the brief outlook is given to reach a complete model that can be used in industry.

4.2 Modeling Framework

4.2.1 Overview

In this modeling approach, the pre-processed tabulated chemistry is coupled to online turbulent flow field calculations in a variable computational domain. 3D CFD simulations are performed with the commercial CFD code STAR-CD and chemistry tables are coupled using user defined functions. The additional transport equations are solved with the CFD code for the defined scalars which serve as look-up variables for interpolations of desired quantities from the tables. Thus, the complex chemistry and turbulent flow calculations are de-coupled to achieve the computational efficiency in these engine cycle simulations. The main aspects of this approach that are different from the previous approach for the constant volume combustion chamber studies (in Chapter 3) is the extension of the FGM table dimensions to include the variable in-cylinder conditions, and the calculation of temperatures using the species mass fractions obtained from the tables. The complete modeling framework can be depicted as in Figure 4.1. The details of these CFD online calculations, pre-processing, and coupling is discussed in further sub-sections.

4.2.2 Turbulent flow - Spray modeling

In-cylinder turbulent flow is modeled using Reynolds Averaged Navier Stokes (RANS) based standard $k–\epsilon$ approach in STAR-CD (The details of the governing equations are presented in Chapter 2). The default model coefficients are applied. The interaction between the turbulent continuous (gaseous) flow and dispersed (liquid droplets) flow is modeled using the coupled two-phase Lagrangian approach. The spray mixture formation is modeled using sub models from STAR-CD [Sta, 2008]. These models include nozzle flow using modified Max – Planck – Institute(MPI) [Obermeier, 1991, Gosman and Marooney, 1991] model which accounts for the cavitation’s effect on the effective nozzle area calculations, droplet break-up and atomization using Reitz – Diwakar [Reitz and Diwakar, 1986] models, inter-droplet collisions using O’Rourke [O’Rourke, 1981] model, wall-droplet interactions using Bai’s [Bai and Gosman, 1995] spray impingement models, and for other interaction processes such as turbulence dispersion, drag, heat and mass transfer by using
the standard correlations from STAR-CD. This combination of sub-models is obtained after an extensive validation study against the non-reacting spray characteristics of Spray H, and Spray A from ECN [ECN, 2012] which was presented in Chapter 3.

**Figure 4.1:** Schematic representation for pre-processing and CFD-FGM online interaction.

### 4.2.3 Chemistry preprocessing

**Laminar chemistry database**

For generating the FGM database, a reduced surrogate gasoline (n-heptane/i-octane/toluene/ethanol) detailed reaction mechanism is used. This mechanism from Andrae [Andrae, 2008] consists of 137 species with 633 reactions. However for NO\(_x\) modeling purpose, it is extended with NO\(_x\) sub mechanism of GRI3.0 resulting in a final mechanism with 152 species and 739 reactions. One of the major advantages with tabulation methods like the FGM approach is that the use of detailed mechanisms involves only a minor cost during the preprocessing stage and with no additional cost during online simulations.

As earlier mentioned, two canonical systems have been defined to generate the databases; one is the ICDF for representing chemistry in the conventional injection strategy, and the other is HR believed to be more representative for the situation during early injection timings. It is to be noted here that details of the boundary conditions that account for the varying in-cylinder conditions for pressure and enthalpy will be discussed in the corresponding sections in this chapter. Only the general details of database generations are presented below. Although they were discussed in earlier chapters, for matter of convenience they are presented here again.

*Igniting Counterflow Diffusion Flames (ICDF)*

The conventional diesel combustion process is predominantly characterized by diffusion
like flames around the spray periphery. And, based on the flamelet theory, the turbulent flame structure can be represented by an ensemble of laminar flamelets. Hence, in this ICDF approach, a set of one-dimensional counter flow diffusion flames is solved with in-house code CHEM1D [Somers, 1994 CHEM1D, 2012]. In a counter flow setup, the oxidizer and fuel streams are considered as two opposing streams which move towards each other and react in a thin region close to the stoichiometric mixture plane. The set of governing equations (2.40 to 2.43) that describes the counter flow diffusion flame is solved, for both igniting and stationary situations to cover the entire regime of diesel combustion. Thus, the composition space of the table has two parts; one is an igniting part and the other is a stationary part. The igniting part is covered with igniting flames which are obtained by solving time dependent equations starting from an adiabatic mixing frozen state solution to a steady state at a single strain rate, typically 500 \( s^{-1} \) (Here, the strain rate is defined as the partial derivative of the flow velocity in the normal direction to the flow, in a counter flow setup). Furthermore, the stationary part is covered with steady flames at different strain rates starting from 500 \( s^{-1} \) to 1.0 \( s^{-1} \). The final solution is approaching chemical equilibrium (see Figure 4.2). In the earlier Chapter 3, it has been validated that igniting flames at a single strain rate can model strain dependency on ignition delay, particularly at lower strain rates.

The detailed chemistry solutions (of igniting and stationary flames) are obtained in time and spatial coordinates. These coordinates are subsequently transformed into two control variables i.e. mixture fraction \((Z)\) and progress variable \((Y)\). The mixture fraction definition is adopted from [Bilger et al., 1990]. The progress variable \((Y)\) 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, with the definition of \(Y\) as:

\[
Y = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{HO_2}}{M_{HO_2}}.
\] (4.1)

Here, \(Y_i\) and \(M_i\) are the mass fraction and molar mass of species \(i\), respectively. The inclusion of \(HO_2\) represents the start of the ignition, \(CO\) represents the intermediate part which subsequently ends with \(CO_2\). The definition of progress variable will not affect results as long as the chemistry parametrization (selection of species) can represent each stage of chemistry evolution.

Subsequently 2D laminar tables are constructed using ICDF chemistry data, based on the two control variables \((Z, Y)\) with 101 points in each dimension. The distribution in the mixture fraction space is equidistant while it is non-equidistant (i.e. quadratic) in the progress variable space.

**Homogeneous Reactors (HR)**

In the HR approach, the 2D manifold is generated using homogenous reactors, i.e. simplified zero-dimensional reactive systems. Here, diffusion and transport are not present, which is a fundamental difference from ICDF. A complete series of HR is computed that together span the same range in mixture fraction space. The initial conditions of the HR are defined
by the adiabatic mixing line, which is also the initial condition of the ICDF database (Figure 4.2). 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. Then again, 2D laminar tables are constructed with a table resolution of 101 points in each dimension, and quadratic spacing for progress variable.

![Figure 4.2: Illustration of temperature as a function of mixture fraction for ICDF, HR, and mixing line.](image)

**PDF integration**

The effect of turbulence on chemistry is taken into account by using a presumed PDF approach. The quantities in the 2D table are integrated with a $\beta$-PDF which is a function of the mean and variance of $Z$ and a $\delta$-PDF function for the mean of $\mathcal{Y}$. When $Z$ and $\mathcal{Y}$ are assumed statistically independent, the mean quantities are defined as,

$$
\tilde{f}(\tilde{Z}, \tilde{Z}''^2, \tilde{\mathcal{Y}}) = \int_0^1 \int_0^1 f(Z, \mathcal{Y}) P(Z || \tilde{Z}, \tilde{Z}''^2) P(\mathcal{Y} || \tilde{\mathcal{Y}}) dZ d\mathcal{Y},
$$

(4.2)

After PDF integration, a 3D table is obtained for a defined boundary condition. The final FGM table resolution which is used here is the best FGM table resolution obtained based on earlier studies found for Spray H of ECN database [ECN, 2012] from Chapter 3, i.e. 101 x 9 x 101(quad) in $\tilde{Z} \times \tilde{Z}''^2 \times \tilde{\mathcal{Y}}$.

**4.2.4 CFD-FGM Interaction**

The coupling between the CFD code and the pre-processed FGM is summarized in Figure 4.1. At each solver time step, the desired quantities are retrieved from the tables for the corresponding five look-up control variables, i.e., $\tilde{Z}, \tilde{Z}''^2, \tilde{\mathcal{Y}}, p, \tilde{h}_{ox}$. Here $h_{ox}$ is oxidizer.
enthalpy, and for adiabatic simulation \( h_{ox} \) is a unique function of \( p \). The first three control variables (i.e. \( \tilde{Z} \), \( \tilde{Z'}_2 \), \( \tilde{Y} \)) are obtained by the additional scalar transport equations that are solved next to mass- and momentum-conservation equations in STAR-CD. They are given now,

Transport equation for \( \tilde{Z} \):

\[
\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z}) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i\tilde{Z}) - \frac{\partial}{\partial x_i}\left[\bar{\rho}(D + D_T)\frac{\partial \tilde{Z}}{\partial x_i}\right] = \tilde{Z}_{spray}, \tag{4.3}
\]

The source term \( \tilde{Z}_{spray} \) from droplet evaporation during spray formation, internally in the STAR-CD solver, acts as a source of the mixture fraction(\( Z \)) equation. The \( D \) and \( D_t \) are the laminar and turbulent diffusion coefficients, respectively.

Transport equation for \( \tilde{Z'}_2 \):

\[
\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z'}_2) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i\tilde{Z'}_2) - \frac{\partial}{\partial x_i}\left[\bar{\rho}(D + D_T)\frac{\partial \tilde{Z'}_2}{\partial x_i}\right] = 2\bar{\rho} \left[ D_T \left( \frac{\partial \tilde{Z}}{\partial x_i} \right)^2 - \frac{\varepsilon}{\kappa} \frac{\partial \tilde{Z'}_2}{\partial x_i} \right], \tag{4.4}
\]

Transport equation for \( \tilde{Y} \):

\[
\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i\tilde{Y}) - \frac{\partial}{\partial x_i}\left[\bar{\rho}(D + D_T)\frac{\partial \tilde{Y}}{\partial x_i}\right] = \tilde{Y}. \tag{4.5}
\]

The source term for the progress variable is retrieved from the pre-tabulated chemistry database. The influence of the variance of \( \tilde{Y} \) is neglected, by assuming a \( \delta \)-function of \( \tilde{Y} \).

Next, the absolute pressure (\( p \)) is directly obtained from the CFD solver. The transported enthalpy scalar (\( h \)) from the CFD solver accounts the effects of heat loss. This static enthalpy is also known as the chemico-thermal enthalpy (equation 2.4). However, this enthalpy variable cannot be directly used to define the boundary conditions of the flames generation during the FGM tabulation process but the values at the boundaries of the flamelets, i.e. \( h_{ox} \) and \( h_{fuel} \) are needed. For a non-adiabatic case, due to the wall heat losses, the oxidizer enthalpy (\( h_{ox} \)) changes at a given pressure level. The effect of wall heat losses on \( h_{fuel} \) is relatively small and neglected, as the fuel vapor stays away from the walls, and the effect due to compression and expansion on \( h_{fuel} \) is negligible. Hence, \( h_{ox} \) is recognized as the only look up variable for heat loss.

For an adiabatic combustion event (with no preferential diffusion i.e. \( Le = 1 \)), the static enthalpy scalar (\( h \)) and the mixture fraction (\( \tilde{Z} \)) are related in a linear way. Therefore, the following expression can be used to extrapolate the oxidizer enthalpy (\( h_{ox} \)), at a given pressure level, from the known static enthalpy (\( h \)), mixture fraction (\( \tilde{Z} \)) obtained from the CFD solver and the (fixed) fuel enthalpy [Nakov et al., 2009].
\[ h_{ox} = \frac{h - h_{fuel} \cdot Z}{1 - Z} \] (4.6)

The same expression (equation 4.6) is used in a non-adiabatic case to derive multiple \( h_{ox} \) values using known values for \( h, Z \) and (fixed) \( h_{fuel} \), which is described more detail in Section 4.5.

Thus all the five required lookup variables are obtained from the CFD solver. More details of table generation for single and multi level \( h_{ox} \), at multiple pressure levels are presented in Sections 4.4.1 and 4.6.1 respectively. Note that a \( \delta \)-function is applied as PDF for \( h_{ox} \) i.e. the effect of \( h_{ox} \) variances is neglected. In the CFD solver, the temperature \( \tilde{T} \) is calculated from the transported scalar enthalpy \( \tilde{h} \) and the species mass fraction distribution \( \tilde{Y}_i \), by using the following expression

\[ \tilde{h} = \sum_{k=1}^{N_s} \tilde{Y}_k h_k(\tilde{T}) \] (4.7)

So, for the purpose of calculating temperature during the CFD computation, the PDF integrated mass fractions of some defined additional species in the CFD solver are also retrieved from the FGM database, in addition to the source of progress variable. As there is a limit to the maximum number of species/scalars in STAR-CD, in a preliminary analysis, the most relevant species are selected based on their contribution (through the formation enthalpy) for computing the temperature. These selected species are considered as ‘active’ scalars in order to account for the mixture properties calculations in STAR-CD.

The retrieval of the desired quantities against the look-up variables from the pre-tabulated chemistry database is performed via a user defined function in STAR-CD.

4.3 Models setup for validation

In this section, the initial model setup for engine cycle simulation is presented. The key inputs for the initial model setup are the engine data (which includes the engine and injection specifications and operating conditions) and the computational grid. These details are described here.

4.3.1 Engine data

Two different operating conditions from two different engine configurations were chosen in this work for validating the model performance for conventional and early injection cases, respectively. The description of the conditions is defined as CDC and PCCI in Table 4.1. For CDC case, a full load operating point (with baseline injection) of a DAF MX engine which is a 6-cylinder Heavy Duty Direct Injection (HDDI) engine that represents conventional injection conditions is considered. And, for PCCI case, a typical low load point of a single cylinder research engine (Cyclops [Leermakers et al., 2011]) which represents early injection conditions is chosen. The Cyclops is based on an earlier DAF engine platform.
Table 4.1: Engine specification and operating conditions chosen for validation of models.

<table>
<thead>
<tr>
<th>Operating conditions</th>
<th>CDC</th>
<th>PCCI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Description</td>
<td>6 cylinder HDDI engine</td>
<td>1 cylinder research engine</td>
</tr>
<tr>
<td>Stroke [mm]</td>
<td>165</td>
<td>158</td>
</tr>
<tr>
<td>Bore [mm]</td>
<td>130</td>
<td>130</td>
</tr>
<tr>
<td>Connecting Rod [mm]</td>
<td>262</td>
<td>266.7</td>
</tr>
<tr>
<td>Compression ratio [-]</td>
<td>16.6</td>
<td>12.0</td>
</tr>
<tr>
<td>Speed [rpm]</td>
<td>1500</td>
<td>1200</td>
</tr>
<tr>
<td>Intake valve closing (IVC) [°CA aTDC]</td>
<td>-120</td>
<td>-153</td>
</tr>
<tr>
<td>Injection timing [°CA aTDC]</td>
<td>-13</td>
<td>-40</td>
</tr>
<tr>
<td>Injection duration [°CA]</td>
<td>36.7</td>
<td>6.5</td>
</tr>
<tr>
<td>Injected mass [g/stroke/cyl]</td>
<td>0.28</td>
<td>0.05</td>
</tr>
<tr>
<td>EGR rate [%]</td>
<td>0</td>
<td>50</td>
</tr>
<tr>
<td>Fuel</td>
<td>Diesel</td>
<td>n-heptane</td>
</tr>
</tbody>
</table>

4.3.2 Computational grids

![Figure 4.3: Sector mesh for CDC (left) and PCCI (right).](image)

The sector grids used, in this work, for CDC and PCCI are shown in Figure 4.3. The grid for the PCCI case looks similar to that of the CDC, except for the differences in the stroke length and squish height, and a slight change in cell size of the moving mesh to match
the lower compression ratio of the research engine. The average cell size ranges from ∼ 1 \( \text{mm} \) and becomes coarser near the cylinder head to ∼ 2 \( \text{mm} \).

### 4.3.3 Initial cycle settings

The engine cycle simulations start at the Intake Valve Closing (IVC) position where the initial conditions are imposed for the pressure, temperature and swirl. The solver time step is controlled with variable steps ranging from 0.25°CA to 0.025°CA, with refined time steps during the injection, ignition and combustion phase.

Periodic boundary conditions are applied to both symmetric planes of the sector grid whereas other planes are treated as walls. The thermal boundary conditions of the cylinder walls, head, and piston are specified as a fixed temperature boundary condition - \( T_{\text{piston}} \) and \( T_{\text{head}} \) equaling 450 K and \( T_{\text{cylinder}} \) equal to 400 K. These values are based on preliminary studies performed using GT-POWER which is a 1D tool for cycle simulations. Note that the heat loss due to radiation is neglected.

The fuel injection rate obtained from experiments is provided as an input using a profile for the CDC case and a fixed rate for the PCCI case. Figure 4.4 shows the plot of fuel injection rates.

![Figure 4.4: Profiles for fuel injection rates vs. CA for CDC and PCCI case.](image)

### 4.4 Pressure dependent FGM for CDC - PCCI

The model is extended with pressure as an additional dimension to FGM. The Pressure dependent FGM influence on the combustion characteristics is studied for two cases i.e. CDC and PCCI cases. The influence of change in pressure (and corresponding adiabatic oxidizer temperature) during the compression stroke on the chemistry is included by considering multiple FGM tables at different pressure levels. The pressure is included as additional look
up variable. The details of the tabulation, CFD implementation and results for both the cases are presented here.

### 4.4.1 FGM tabulation

Empirical pressure levels are chosen from known experimental pressure traces, during pre-processing of the chemistry database. The effect of heat loss on the chemistry evolution is neglected in the model. Hence each pressure level is linked with a corresponding (i.e. adiabatic) oxidizer temperature or enthalpy that defines the oxidizer boundary condition for the FGM table.

![Chart showing pressure and temperature relationship](chart.png)

**Figure 4.5:** The experimental cylinder pressure trace (in blue) and temperature (in green). The chosen pressure levels and corresponding oxidizer temperatures between SOI and peak cylinder pressure are shown with dotted lines.

![Diagram illustrating temperature and enthalpy boundary conditions](diagram.png)

**Figure 4.6:** Illustration of the temperature and enthalpy boundary conditions for 1D counter flow steady flames at three different pressures.

For the CDC case, 7 pressure levels are selected (equi-distant in logarithmic space)
ranging between a pressure at around start of injection (10.7 MPa) and the peak cylinder pressure (18.2 MPa) as shown in Figure 4.5. The corresponding gas temperature from the experimental data defines the oxidizer temperature while the fuel side temperature is fixed to the initial fuel injection temperature. Since it is a non-EGR condition, the oxidizer is assumed to be pure air. As mentioned earlier, ICDF are used to generate the chemistry tables at each pressure level. To illustrate the boundary conditions, steady counter flow diffusion flames (adiabatic) with applied strain rate of \(500 \text{ s}^{-1}\) for three pressure levels \(P_1, P_3\) and \(P_7\) are shown (see Figure 4.6). The \(T_{ox}(p)\) and derived \(h_{ox}(p)\) values at the boundary are marked. It is to be noted that a linear relation exists between enthalpy \((h)\) and mixture fraction \((Z)\) for an adiabatic flame. However in case of heat loss this is formally no longer valid.

For the PCCI case, 5 arbitrarily chosen pressures are considered, ranging between the pressure at end of injection (1.5 MPa) and the pressure close to the end of rapid combustion (5.25 MPa). The corresponding temperature (or enthalpy) conditions are estimated in a similar way as for the ICDF’s case. Since HRs are used for chemistry tabulation in the PCCI case, the initial conditions are obtained by the adiabatic mixing line which is defined by boundary conditions for the corresponding pressure level. The mixture composition at oxidizer side is defined based on 50% EGR.

4.4.2 Results: Conventional injection case (CDC)

To validate the FGM and evaluate the effect of pressure dependent FGM on the combustion characteristics of a conventional injection case of the DAF MX engine, 4 different simulations are performed. One is with an FGM table based on an average pressure between the pressure at Start of Injection (SOI) and peak cylinder pressure, and others are with 3, 5, and 7 pressure levels in the same range. (Here, the conditions for the average pressure case are \(p=15.2 \text{ MPa}, T_{oxidizer} = 937 \text{ K}, T_{fuel} = 353 \text{ K}\). First the auto-ignition delay predictions are compared, and then the rest of the heat release rate spectrum is studied.

In this study, the auto-ignition delay is defined as the time duration between the Start of Injection (SOI) and the time at which the positive rise of the cumulative heat release occurs (can be referred to as start of combustion, SOC) after the cooling effect due to evaporating fuel and heat loss to walls. Figure 4.7(left) shows the comparison of the cumulative heat release predictions from the models against experimental data, mainly focusing around the point of ignition. The difference in the magnitudes of cumulative heat release between the experiments and the models is mainly due to two factors. The first reason is that the model under-predicts the heat loss to walls (cylinder liner / piston / head) which are fixed at 400 K / 450 K / 450 K based on previous studies (It is important to note here that the FGM table is referred to as the adiabatic, however the simulation is non-adiabatic). The second reason is the difference in heat of evaporation for \(n\)-heptane (316 kJ/kg) and diesel fuel (250 kJ/kg) which leads to a difference in evaporating cooling due to the fuel injection.

The model with one FGM table at a single averaged pressure condition shows early ignition compared to the other models with pressure dependent FGM tables. This is simply due to the fact that the table is generated at a considerably higher pressure and temperature than the actual conditions around ignition. In case of the approach with multiple pressures, FGM tables are generated at conditions around the point of ignition. The source terms re-
Figure 4.7: (left) Comparison of pressure dependence of FGM on ignition delay. (right) Comparison of mean source of progress variable retrieved from the database for the different pressure dependent tables.

Retrieved from the database are consequently much more relevant. The difference between the different implementations can be observed in Figure 4.7(right). There are huge fluctuations observed in these numerical predictions which are mainly due to the stochastic nature of spray droplets injection, subsequent vapor formation and retrieval of source terms from the tables. This figure also shows that the FGM model with 5 pressure levels is sufficient as the source terms collapse with that of the following case. This is consistent with the observations in earlier work [Bekdemir et al., 2011]. Here, the model with pressure dependent FGM shows slightly over-predicted ignition delay. The slight impact of thermal stratification on progress variable source terms, which the current model does not take into effect, can be one of the reasons. This is further explained in Section 4.6.2 Otherwise, the uncertainties in experimental pressure trace and the intrinsic inaccuracies in the \( n \)-heptane mechanism also contribute to this ignition delay deviation.

To evaluate the model predictions during the entire combustion phase, in Figure 4.8, the cylinder pressure, heat release rate, and cumulative heat release predictions from the pressure dependent FGM with 5 pressure levels is compared with the experimental data. The simulation shows rapid rise in heat release and cylinder pressure during ignition compared to experimental data. This deviation is caused by the short burn duration characteristics of the reaction mechanism [Bekdemir, 2012], and the accumulation of a large fuel content (around 200% higher) during the over-predicted ignition delay when compared to that during the time period of actual (experimental) ignition delay in the model. The cumulative heat release rate is over-predicted by the model since the lower heating value of \( n \)-heptane (44.6 MJ/kg) is higher than that of diesel (41.54 MJ/kg), and the model under-predicts the heat loss to the wall as earlier explained. This, in-fact, gives rise to approximately 7% over-prediction in peak cylinder pressure predictions. However, the combustion duration matches reasonably well with experimental data.

Currently the tabulation is not extended into the expansion stroke as we focus on ignition here. Furthermore, it doesn’t account for the influence of heat loss yet, as the tabulation
Figure 4.8: Comparison of averaged cylinder pressure (above), heat release rate (middle) and cumulative heat release (bottom) of FGM model with 5 pressure levels and experimental data.

is performed with adiabatic flames. Their oxidizer temperature is set equal to that of the corresponding gas temperature (as adiabatic) from the experiments. Consequently fuel vapor remnants that will not react due to the expansion cooling and heat loss from the walls are not yet accurately predicted. To account for this, an additional controlling variable, the specific enthalpy (or) enthalpy deficit [Nakov et al., 2009], should be introduced in the tables at each pressure level. This extension is vital before the emission’s model implementation which is presented in Section 4.7 of this chapter.

4.4.3 Results: Early injection case (PCCI)

In case of the early injection study, three simulations are performed with pressure dependent HR based FGMs. Similar to the conventional case study, one is with FGM at an average pressure condition \((p = 4.0 \text{ MPa, } T_{\text{oxidizer}} = 800 \text{ K, } T_{\text{fuel}} = 353 \text{ K})\) and others are with FGMs at 3 and 5 levels of pressures, ranging from the pressure at end of injection and the pressure at around end of rapid combustion. Due to large ignition delay (around 30 °CA) in this early injection case (PCCI like conditions), it is difficult to predict and therefore an important characteristic for the model to capture this accurately. This is much more demanding than in the conventional injection case where ignition delay is only 4 °CA. In Figure 4.9 the cumulative heat release from these simulations has been compared with that from engine experimental data, mostly focusing around the point of ignition. The SOI, EOI and SOC points are indicated in the plot. The model with HR based FGM at the average pressure condition obviously fails to capture the ignition delay. It shows very early ignition,
due to the fact that the tables are generated at a high pressure and temperature condition, giving far more reactive conditions than prior to ignition. With FGM tables at 3 or 5 pressure levels, the model shows a more acceptable ignition delay which agrees well with the experiment. The ignition delay predicted with the 5 pressure level FGM is slightly better than that of the 3 pressure level FGM. Figure 4.10 shows the heat release rates (left) and full cumulative heat release (right) from modeling and experimental data. The HR based FGM model with more pressure levels captures experimental heat release rate in better way, while average pressure based FGM completely fails. However, the model results show a rapid rise in heat release and fail to capture the double rise, due to cool flame combustion phase as seen in experimental data. Eventually, the peak of heat release rates is over-predicted. This is mainly caused by the inherent characteristics of HR which are used for FGM tabulation. They are all single stage igniting systems and insensitive to the flow straining. In the work of [Egüz, 2013], it is found that the use of ICDF based FGM (generated at low strain rate)
shows an improved rise of heat release. However the selection of strain rates to generate igniting flames introduces another modeling uncertainty. It is also to be noted here that the reduced reaction mechanism used has shorter burn duration ($\tau_{80} - \tau_{20}$) around 50% of that of a larger reaction mechanism i.e. from LLNL [Bekdemir, 2012]. This difference corresponds to the observed difference between model (0.83 ms) and experiment (1.94 ms). The

![Figure 4.11: Comparison of averaged cylinder pressure of pressure dependent FGM model with experimental data.](image)

combustion duration is under-predicted by both 3 pressure level and 5 pressure level FGMs. This is caused by the incomplete combustion by these models which can also be observed from the under-predicted (by around 8%) cumulative heat release (Figure 4.10(right)). The rapid rise in heat release and incomplete combustion causes a faster pressure rise and an under-prediction of peak cylinder pressure (by around 8.5%) by the models when compared to the experimental data (see Figure 4.11). The predicted $CO$ from the 5 pressure level FGM model is around 15000 ppm while the experimental value is 4000 ppm. This observation also corroborates the incompleteness of the combustion from the model. The high amounts of $CO$ from the simulations are observed mainly at the crevice regions. Hence the FGM model including heat loss can also be expected to improve the results by interpolating $CO$ from more representative tables.

### 4.5 A-priori study for enthalpy levels in engine cycle simulations

In case of CDC, the heat loss from the flame to the walls may play an important role. Due to the proximity of the piston bowl / cylinder liner / cylinder head walls, the hot diffusion flame loses heat significantly resulting in lower flame temperatures. In order to take the effect of this change in temperature on chemistry into account, a new variable has to be added in FGM to provide information on the local state with respect to heat loss. That variable is oxidizer
enthalpy \((h_{ox})\) which is connected to the static chemico-thermal enthalpy, \(h\) (equation 4.6). Since this static enthalpy is a conservative scalar which is transported, it does take into account of the heat loss in in-cylinder flow simulations. The transport equation for the static enthalpy in CFD solver is as follows:

\[
\frac{\partial}{\partial t}(\bar{\rho}\tilde{h}) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{h}) = \frac{\partial}{\partial t}\bar{p} + \bar{u}_i\frac{\partial}{\partial x_i}\bar{p} - \frac{\partial}{\partial x_i}(\tilde{q}_i + \bar{\rho}\tilde{u}_i''\tilde{h}'') + \tau_{ij}\frac{\partial u_i}{\partial x_j} + \tilde{S}_h, \tag{4.8}
\]

where \(\tilde{q}_i\) is diffusion energy flux and \(\tilde{S}_h\) is energy source.

The extension of the FGM table with enthalpy as additional dimension for engine cycle simulations has many challenges. The main challenge is determining the range of the enthalpy levels that have to be included. Hence, an a-priori study is performed to determine which levels are to be considered for FGM generation. Two CFD simulations with 5 pressure and 1 enthalpy level FGM for the CDC case are performed, one is with non-adiabatic CFD and the other is with adiabatic CFD conditions. The latter is imposed by applying adiabatic boundary conditions to the piston bowl, cylinder liner and cylinder head walls. The static enthalpy data at different CA positions from these two simulations is studied.

**Figure 4.12:** Scatter plots of static enthalpy vs. mixture fraction for non-adiabatic simulation (left) and adiabatic simulation (right) for the CDC case with 5 pressure level FGM. The blue dashed lines indicate the enthalpy data from earlier introduced FGM at 5 pressure levels.

In Figure 4.12, the enthalpy scatter data is depicted for a few CA positions being 709°CA, 720°CA (i.e. TDC), 740°CA and 760°CA for both simulations. The enthalpy data from the flames used for FGM tables at different pressures are also included in blue dashed lines. It is to be noted here that injection starts at 707°CA. The reason for the limited range of \(Z\) values around 0.35 is the finite resolution of the computational cells. In Figure 4.12(right), the scatter plot for the adiabatic case shows the expected linear mixing relation between enthalpy and \(Z\) (until 740°CA position) as described in Section 4.2.4. However, the same plot from the non-adiabatic simulation (in Figure 4.12(left)) shows a
cloud of points which deviates from the linear relation, mainly at CA positions of 720°CA (in black), 740°CA (in green). This deviation in \( h(z) \) will be used to estimate the new oxidizer enthalpy \( (h_{ox}) \), using equation (4.61), which corresponds to a certain level of heat loss. These oxidizer enthalpy conditions (at \( Z = 0 \)) are used for the flamelet calculations while the fuel enthalpy conditions (at \( Z = 1 \)) remain fixed for all cases.

However, it is important to note here that the above consideration is only valid until the post combustion event starts, i.e. generally after the end of the injection event (in this case, it is 745°CA). This is because, for these expansion phase conditions, the FGM tables cannot be generated using an ‘igniting’ flamelet since the corresponding ICDF would involve cryogenic fuel temperature and a too low oxidizer temperature such that it never ignites. Possible ways to circumvent this problem is specifying

- Igniting Counterflow Partially Premixed flames for various \( h_{ox}/h_{pp} \) conditions observed. \( h_{pp} \) is the corresponding enthalpy at partially premixed fuel side i.e. the rich side \( (Z < 1) \).

- Burning Counterflow Partially Premixed flames. Extract the solutions after EOI (sample/extract ‘flamelets’ from the ‘active’ \( Z, Y \) part of the FGM tables) and let them cool down to a series of given pressure and variations of \( h_{ox}/h_{pp} \) observed.

- Set of homogeneous reactor solutions initiated with conditions from the solution after EOI and let them cool down to given set of pressure and enthalpy \( (h_{ox}/h_{pp}) \) conditions.

Since the main focus of the current study is to account of heat loss influences on the chemistry during the main combustion event, the tables are considered only until the post combustion event.

Now the range of oxidizer enthalpy values for each pressure value from CFD simulation is estimated. The obtained oxidizer enthalpy values at a given pressure level are the new flamelet parameters which take into account of the cooling effect. In Figure 4.13, the maximum and minimum values of oxidizer enthalpy are plotted at various CA position along with experimental cylinder pressure data. At each pressure level, the appropriate range of \( h_{ox} \) is used to extend the FGM tables. It is also observed that this range is not dependent on the combustion model used for these simulations (since the static enthalpy does not change due the course of combustion, rather it is majorly influenced by the heat loss). Same minimum \( h_{ox} \) is chosen since all the values are almost same for all pressures, while the maximum values of oxidizer enthalpy are picked encompassing entire range of \( h_{ox} \) spread at corresponding pressure value. 5 levels of \( h_{ox} \) with equidistant spacing are considered at each pressure level and the corresponding oxidizer temperatures are obtained, which are given in Table 4.2. The data values in bold are the oxidizer enthalpies (corresponding to pressures) used in Pressure dependent FGM case, which are obtained directly from the average in-cylinder temperature trace (see Section 4.4.1). The details of table generation and complete implementation of Pressure and Enthalpy dependent FGM for conventional injection case (CDC) is presented in the next section.
In this section, the Pressure dependent FGM model is extended with enthalpy as an additional dimension for CDC case. The effect of heat loss on chemistry is incorporated by generating multiple FGM tables at different oxidizer enthalpy levels in-addition to the adiabatic enthalpy level for the corresponding pressure. The additional look-up variable $h_{ox}$ extracted from the CFD solver for a computational cell (as explained in Section 4.2.4) will be used to interpolate the desired quantities (for sources, species mass fractions) from the FGM database. This is now much more corresponding to local temperature of the cell, when compared to that in case of only Pressure dependent FGM.

The effect of Pressure and Enthalpy dependent FGM on the global combustion characteristics and local flame structures are studied. The details are presented here.

### 4.6.1 FGM tabulation

During the preprocessing step, for ICDF generation, 5 moderate pressure levels are selected in the range from start of injection to the peak cylinder pressure, from the experimental trace. At each pressure level, 5 levels of oxidizer enthalpy conditions are included. The oxidizer enthalpy (temperature) boundary conditions are obtained from a-priori study, as explained in Section 4.5, where enthalpy data from CFD is used to extrapolate the oxidizer enthalpy. The multiple oxidizer enthalpy (temperature) conditions for corresponding pressures are
Table 4.2: Engine specification and operating conditions chosen for validation of models.

<table>
<thead>
<tr>
<th>Pressure</th>
<th>$h_{ox_{min}} - h_{ox_{max}}$</th>
<th>$h_{ox_{1}}(T_{ox_{1}})$ kJ/kg (K)</th>
<th>$h_{ox_{2}}(T_{ox_{2}})$ kJ/kg (K)</th>
<th>$h_{ox_{3}}(T_{ox_{3}})$ kJ/kg (K)</th>
<th>$h_{ox_{4}}(T_{ox_{4}})$ kJ/kg (K)</th>
<th>$h_{ox_{5}}(T_{ox_{5}})$ kJ/kg (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_1$</td>
<td>4.72 - 5.84</td>
<td>4.72 (750)</td>
<td>5.00 (775.7)</td>
<td>5.28 (801.1)</td>
<td>5.56 (826.4)</td>
<td>5.84 (851.0)</td>
</tr>
<tr>
<td>$P_2$</td>
<td>4.72 - 6.21</td>
<td>4.72 (750)</td>
<td>5.09 (784.1)</td>
<td>5.46 (817.8)</td>
<td>5.84 (851.0)</td>
<td>6.21 (884.0)</td>
</tr>
<tr>
<td>$P_3$</td>
<td>4.72 - 6.40</td>
<td>4.72 (750)</td>
<td>5.14 (788.5)</td>
<td>5.56 (826.4)</td>
<td>5.98 (864.0)</td>
<td>6.40 (901.3)</td>
</tr>
<tr>
<td>$P_4$</td>
<td>4.72 - 8.08</td>
<td>4.72 (750)</td>
<td>5.56 (826.5)</td>
<td>6.04 (901.3)</td>
<td>7.24 (975.1)</td>
<td>8.08 (1047.8)</td>
</tr>
<tr>
<td>$P_5$</td>
<td>4.72 - 8.08</td>
<td>4.72 (750)</td>
<td>5.56 (826.5)</td>
<td>6.40 (901.3)</td>
<td>7.24 (975.1)</td>
<td>8.08 (1047.8)</td>
</tr>
</tbody>
</table>

Figure 4.14: Illustration of steady counter flow diffusion flames used to construct FGMs for 5 oxidizer enthalpy levels at $P_3$ pressure level (left). The zoomed region to illustrate the oxidizer levels (right). The typical CFD scatter data is shown in black dots.

shown in Table 4.2. To illustrate these ICDF at multiple oxidizer enthalpy conditions, the enthalpy vs. mixture fraction plots for 5 oxidizer enthalpy level ICDF are shown for a given pressure level, for instance $P_3$, in Figure 4.14. Now, the final FGM table resolution becomes 5 x 5 x 101 x 9 x 101 in the directions $p, \tilde{h}_{ox}, \tilde{Z}, \tilde{Z}'^2$ and $\tilde{Y}$, respectively. This extended chemistry database is coupled to the CFD solver.

4.6.2 Results: the effect on engine combustion characteristics

The simulation with the Pressure and Enthalpy dependent FGM is performed for CDC case and the results are compared with that from simulations with Pressure dependent FGM. The Pressure and Enthalpy dependent FGM model is referred to as $FGM_{ph}$ and pressure dependent FGM is referred to as $FGM_p$. 
The pressure traces and heat release rates from the two simulations and experimental data are shown in Figure 4.15(left) and Figure 4.15(right), respectively. From heat release rate, it can be observed that the $FGM_{ph}$ (in green) shows a slight advancement of the start of combustion when compared to $FGM_p$ (in black), however the effect is minimal. A minor improvement is also noticed for the initial premixed heat release rate as the over-prediction of the peak value is less.

This is investigated in more detail. In Figure 4.16, the distribution of $h_{ox}$ (due to heat loss) retrieved from the CFD analysis is presented. The single $h_{ox}$ used with the $FGM_p$ approach is also presented and indicated with a red line (see also table 4.2). Up to ignition the distribution is rather mono-disperse indicating the minor effect of heat-loss prior to the combustion event. In Figure 4.17, the retrieved source terms of the progress variable are presented for both FGM tables are given. The fact that the $FGM_{ph}$ contains higher $h_{flamelet}$ states, as shown in 4.17 reflect itself in the higher source terms and consequently earlier ignition. The fact that the ignition is slightly earlier reduces the premixed fraction of the CDC event which on its turn explains the lower pre-mixed spike observed in Figure 4.15.

During the diffusion combustion phase (CA>720), the predicted pressure and heat release rates are relatively higher for $FGM_{ph}$ when compared to $FGM_p$. This is not expected, as the $FGM_{ph}$ accounts for the heat loss and it should result in lower CFD temperatures and lower pressures (heat release rates). To investigate further, the CFD temperatures and database (flamelet) temperatures are compared between the two models (in Figure 4.18). The CFD temperatures from $FGM_{ph}$ is slightly higher than that from $FGM_p$, but what is important to realize now is that the $FGM_{ph}$ database temperature corresponds to the CFD temperature which was not the case for the $FGM_p$. This is simply due to the fact that $FGM_{ph}$ has an additional dimension to interpolate flamelet temperatures from more relevant tables (for that corresponding CFD temperature). Whereas, in case of $FGM_p$, since only single table exists for enthalpy (temperature) condition which is (mostly) different.

**Figure 4.15:** Comparison of cylinder pressure trace (left) and heat release rate trace (right) results from model with $FGM_p$, and $FGM_{ph}$ with experimental data.
Figure 4.16: Distribution of estimated oxidizer enthalpy \( (h_{ox}) \) at various pressure levels of interest. The marked red dotted line shows the single (adiabatic) enthalpy considered in FGM\(_p\) model.

Figure 4.17: The scatter plots for source terms of \( Y \) and flamelet enthalpy against \( Z \) space, when piston is at different CA positions of interest. The simulation data from both models is compared, where FGM\(_{p}\) is shown in black, FGM\(_{ph}\) is shown in green.

from CFD temperature. Mathematically, it refers that the ability of the model to interpolate
from more relevant databases. Moreover, during next time steps, the CFD temperature is calculated using the transported static enthalpy from CFD and the mixture composition data ($Y_i$) retrieved from the FGM tables (equation 4.7). Since, $FGM_{ph}$ model results in more relevant $Y_i$ retrieved from tables the CFD temperature predictions are more accurate than that from $FGM_p$ models. Although these differences in temperature predictions doesn’t show major impact on ignition delay and global pressure/HRR traces it will be much more relevant for $NO_x$ emissions simulations which will be explained in Section 4.7.

![Figure 4.18: Comparison of in-cylinder average CFD temperatures with the average flamelet temperature in crank angle space, for two models $FGM_{ph}$ and $FGM_p$.](image)

**4.6.3 Results: the effect on flame structure**

The effect of the enhanced FGM model on local flame structures is visualized with the help of the predicted local $OH$ fields. In Figure 4.19, the contours of $OH$ at four different CA positions starting from 712°CA and with spacing of 10°CA are plotted for $FGM_p$ on left and $FGM_{ph}$ on right, respectively. It is one of the fundamental advantages of the FGM approach that it can render scalar fields of intermediate species which are of interest. Due to the slight advancement in ignition, in case of $FGM_{ph}$, the flame appears at 712°CA position earlier when compared to $FGM_p$ case. Further, the onset of the flame is quite comparable for the two cases. However, the peak concentration of $OH$ when the flame reaches the vicinity of the walls is considerably reduced in case of $FGM_{ph}$. This shows that the chemistry from $FGM_{ph}$ model is altered by the effect of heat loss. Especially at 742°CA position, it is observed that there is a huge reduction ($\sim 25\%$) in the localized peak $OH$ concentrations, close to the piston bowl and cylinder head. It can be inferred from these observations that the additional dimension in FGM model is able to account for the effect of the cooling on the evolution of intermediate species, and consequently predict emissions more accurately. In the next section, the $NO_x$ model implementations in this improved FGM model are presented.
4.7 Effect of the model enhancements on $NO_x$ prediction

Since the kinetics of Nitrogen oxides, $NO_x$ (both NO and $NO_2$) formation in diesel engine combustion is highly dependent on the temperatures and gas mixture distribution, the improvements due to model enhancements can be quantified based on these $NO_x$ predictions. In this section, first a short description of $NO_x$ formation mechanisms is provided. Then the $NO_x$ model implementation is described and the model predictions are discussed.

Nitric oxide ($NO$) is typically the major contributor to the total $NO_x$ produced in diesel engines, the nitrogen dioxide ($NO_2$) contribution ranges from 10-30% and it is especially more prominent at low load and low speed operating conditions of diesel engines [Heywood, 1988 Stiesch, 2003]. The $NO$ formation can originate from the $N_2$ present either in ambient air or in fuel. Since diesel fuel contains insignificant levels of fuel bound $N$, the fuel $NO$ formation is generally not considered. The mechanisms for $NO$ formation due to $N_2$ in ambient air are the Thermal $NO$ (Zeldovich $NO$), Prompt $NO$, and $N_2O$ intermediate pathway. Thermal $NO$, as the name indicates, forms at high temperatures via oxidation of Nitrogen molecules with $O$, $O_2$, and $OH$ present in the mixture composition. Many of the studies consider partial equilibrium approximations for $O$, $OH$, and steady state assumption for $N$ due to the limitation of details in simplified combustion models. Prompt $NO$ occurs mainly in fuel rich regions of the flame due to reactions between $N_2$ and the hydrocarbon radicals such as $C_2$, $C_2H$, $CH$, and $CH_2$ forming $HCN$ which fur-
ther reacts to \( NO \). As the resolved radical concentrations are required for this mechanism, the detailed chemistry is needed although the contribution of this pathway is only around 5-20% to total \( NO \) formation. The third mechanism is the leading intermediate pathway where the similar (first) reaction of thermal \( NO \) occurs at relatively low temperatures to \( N_2O \) instead of \( NO \). On the other hand, \( NO_2 \) formation is due to the reaction between \( NO \) and \( HO_2 \) occurring at the flame zone. Mostly this \( NO_2 \) converts back to \( NO \) by reacting with \( O, H \) depending on the local conditions.

### 4.7.1 \( NO_x \) modeling

In this study, two different approaches are adopted in FGM to model \( NO_x \) formation. Both approaches solve an additional transport equation with different models for its source terms. The details of two different approaches are presented here.

1. Estimated source approach: In this approach only thermal \( NO \) is consider in the model. The transport equation for \( NO \) reads as,

\[
\frac{\partial}{\partial t}(\bar{\rho} \bar{Y}_{NO}) + \frac{\partial}{\partial x_i}(\bar{\rho} \bar{u}_i \bar{Y}_{NO}) - \frac{\partial}{\partial x_i} \left[ (\bar{\rho} (D + D_T) \frac{\partial \bar{Y}_{NO}}{\partial x_i}) \right] = \dot{\bar{NO}},
\]

(4.9)

The source terms \( \dot{\bar{NO}} \) are calculated as a post-processing step using the extended Zeldovich mechanism. The given net rate from the thermal \( NO \) mechanism [Heywood, 1988] is,

\[
\dot{\bar{NO}} = \frac{d\bar{NO}}{dt} \approx k_1(\bar{T})[\bar{N}_2][\bar{O}] + k_2(\bar{T})[\bar{N}][\bar{O}_2] + k_3(\bar{T})[\bar{OH}][\bar{N}]
\]

\[
-k_{-1}(\bar{T})[\bar{NO}][\bar{N}] - k_{-2}(\bar{T})[\bar{NO}][\bar{O}] - k_{-3}(\bar{T})[\bar{NO}][\bar{H}].
\]

(4.10)

where \( k_1, k_2, k_3 \) (forward reaction rate constants) and \( k_{-1}, k_{-2}, k_{-3} \) (reverse reaction rate constants) are strong functions of temperature (details given in Appendix B). Note that this is the most simplified modeling approach and the method use an implicit choice for the TCI of the \( NO \) source term i.e. \( \dot{\bar{NO}}(\bar{Y}_i) \neq \dot{\bar{NO}}(\bar{Y}_i) \), which formally is incorrect. It is however the common practice in most CFD solvers. For that reason, in the next approach, the direct TCI treated source terms retrieved from the tables are used.

The main step in this approach is to obtain the concentrations for \( N, H, O, \) and \( OH \). The two different methods that are used in this approach to obtain these concentrations are

- By using steady state assumption for \( N \) species and equilibrium approximation for \( O, OH \) radicals. It is a very simple and typical engineering approach. The details of this method are included in Appendix B.
• By retrieval of all relevant radicals directly from the FGM database. The TCI is equal to that of the progress variable. For example, the \( \text{OH} \) radicals retrieved from tables are,

\[
\widetilde{\text{OH}}(\tilde{Z}, \tilde{Z}^n, \tilde{Y}) = \int_0^1 \int_0^1 \text{OH}(Z, Y) P(Z \| \tilde{Z}, \tilde{Z}^n) P(Y \| \tilde{Y}) dZ dY,
\]

(4.11)

2. Tabulated source approach: The same transport equation is solved but for \( \text{NO} + \text{NO}_2 \) (i.e. \( \text{NO} + \text{NO}_2 \)) which is given by,

\[
\frac{\partial}{\partial t} (\bar{\rho} \tilde{Y}_{\text{NO}_x}) + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{Y}_{\text{NO}_x}) - \frac{\partial}{\partial x_i} \left[ \bar{\rho} (D + D_T) \frac{\partial \tilde{Y}_{\text{NO}_x}}{\partial x_i} \right] = \dot{\text{NO}}_x,
\]

(4.12)

Now, mainly the source terms \( \dot{\text{NO}}_x \) are retrieved directly from the FGM database. As mentioned earlier, the \( n \)-heptane oxidation reaction mechanism which is used to generate FGM database is extended with \( \text{NO}_x \) sub-mechanism from GRI 3.0 [Smith et al., 2012]. This includes full \( \text{NO}_x \) kinetics (except fuel \( \text{NO}_x \)). Hence, the obtained source terms include all \( \text{NO}_x \) mechanisms. The TCI during tabulation is equal to that of the similar to source of progress variable, an explicit consistent choice for the TCI namely the \( \beta \)-pdf (see Section 2.3.3).

### 4.7.2 Results: estimated source approach

The thermal \( \text{NO} \) model based on estimated sources (using either steady state/equilibrium radicals or retrieved radicals) is implemented in FGM STAR-CD framework for engine cycle simulation. In order to study the effect of the FGM model enhancements on \( \text{NO} \) predictability, the simulations with \( \text{FGM}_{ph} \) and \( \text{FGM}_p \) are performed and the results are compared. Here, the steady-state/equilibrium radical based \( \text{NO} \) is termed as \( \text{NO} \)\(_{\text{Zeldovich – steadystate}} \) and retrieval radicals based \( \text{NO} \) is termed as \( \text{NO} \)\(_{\text{Zeldovich – detailed}} \).

In Figure 4.20, the mass fraction of \( \text{NO} \) (left) and the corresponding average source terms (right) from both methods are plotted. The predictions from the \( \text{FGM}_p \) and \( \text{FGM}_{ph} \) are compared. It is observed that all \( \text{NO} \)\(_{\text{Zeldovich – steadystate}} \) predictions are comparable as no significant effect is shown due to the improvements in FGM model. It is attributed to the fact that the source terms obtained from steady-state/equilibrium approximation preclude the direct influence of the local radical composition on \( \text{NO} \) formation. And, intriguingly \( \text{FGM}_{ph} \) model shows a slight increase in \( \text{NO} \)\(_{\text{Zeldovich – steadystate}} \) when compared to \( \text{FGM}_p \) model. However, it is not the case with the \( \text{NO} \)\(_{\text{Zeldovich – detailed}} \) predictions. The \( \text{FGM}_{ph} \) model shows a considerable effect due to heat loss on \( \text{NO} \) and slows down the production when compared to \( \text{FGM}_p \) model. It is also evident that the start of \( \text{NO} \)\(_{\text{Zeldovich – detailed}} \) production is advanced by roughly 10°CA, and the magnitudes are higher by 3-4 times when compared to that of \( \text{NO} \)\(_{\text{Zeldovich – steadystate}} \).

In order to investigate the reasons for this further, \( \text{OH} \) (left), \( O \) (right) and their steady-state radicals are compared for the two FGM models as shown in Figure 4.21. Interestingly,
Figure 4.20: Effect of model enhancements on transported NO (left), and source terms (right) based on the extended Zeldovich thermal NO mechanism. The dotted lines refer to steady state method, the solid lines refer to detailed (or radical retrieval) method. $FGM_{ph}$ (in green), $FGM_p$ (in black).

Figure 4.21: Effect of model enhancements on intermediate radicals’ mass fractions of OH, O (solid lines) and their steady state species i.e. $OH_e$ and $O_e$ (dotted lines). $FGM_{ph}$ (in green), $FGM_p$ (in black).
the qualitative trends of the corresponding radicals (in-cylinder average quantities) obtained from steady state and retrieval methods are quite similar. When they are compared quantitatively, the concentrations of steady state radicals are lower compared to that of retrieved radicals.

Figure 4.22: Retrieved/detailed radicals of O(top) and source terms of NO(bottom) from FGM<sub>p</sub> model (left) and FGM<sub>ph</sub> model (right), when piston is at 735ºCA.

This justifies the main reason for the lower production of NO(Zeldovich—steadystate) compared that of NO(Zeldovich — detailed). However, the relative effect of the FGM<sub>ph</sub> on NO(Zeldovich — steadystate) is not comprehensible despite the lower mass fraction of OH<sub>e</sub> and O<sub>e</sub> for the FGM<sub>ph</sub> compared to that from the FGM<sub>p</sub> model. This necessitates looking into the radical’s spatial distribution, and sources between these models to understand the reasons for the differences. In Figure 4.22 and Figure 4.23, the contours of O (or O<sub>e</sub>) radicals (top) and source terms of NO(bottom) are plotted for NO(Zeldovich — detailed) and NO(Zeldovich — steadystate), respectively. The FGM<sub>p</sub> case is plotted on left side and FGM<sub>ph</sub> on right side of the figures. In case of retrieved/detailed radicals based NO, the FGM<sub>p</sub> shows higher O concentration along the entire plume and results in higher production of sources compared to that from the FGM<sub>ph</sub>. Whereas, in case of steady state radicals based NO, the localized concentration of O<sub>e</sub> in the core of the plume contributes to higher production of sources in the FGM<sub>ph</sub>, despite the higher O<sub>e</sub> in other regions in the FGM<sub>p</sub> model which is the reason for the slightly higher average values as shown in Figure 4.23(right, bottom). The similar observations are also found for OH and OH<sub>e</sub> concentrations.

Hence, the major outcomes from this study are
Predicted NO using the Zeldovich mechanism with retrieved values for the radicals is higher compared to that with equilibrium assumptions for the radicals, for all FGM formulations.

The effect of FGM model enhancements are majorly shown only on NO(Zeldovich—detailed), except for a minor effect for FGM\(_{ph}\) in case of NO(Zeldovich—steady state) due to the radicals distribution which favors the NO production.

### 4.7.3 Results: tabulated source approach

Next, the full \(NO_x\) model is implemented based on tabulated source terms in engine cycle simulations. Again, the two simulations (\(FGM_{ph}\) and \(FGM_h\)) are performed to study the effect of the model enhancements on \(NO_x\) predictability. Source terms with and without pdf integration (i.e. integration of \(\beta\)-pdf and \(\delta\)-pdf function for \(Z\), respectively) are applied to evaluate the impact of turbulence and chemistry interaction (TCI) on \(NO_x\) formation. The results till 745\(^\circ\)CA are processed to analyze the impact of model enhancements and also since the post combustion event i.e. after around 745\(^\circ\)CA is not yet implemented in FGM tabulation.

In Figure 4.24, the average \(NO_x\) mass fractions (left) and source terms (right) are compared for two FGM models. Results for both with and without pdf integrated source method are included. The model enhancements have a noticeable impact on the \(NO_x\) formation. The \(FGM_p\) model results in higher sources of \(NO_x\) compared to the \(FGM_{ph}\) model. This stems from the fact that the \(FGM_{ph}\) database \(T\) (i.e. \(T_{flamelet}\)) corresponds to actual \(T\) (i.e. \(T_{CFD}\)) and therefore the stored values of source terms are relevant for the actual condi-
Figure 4.24: Effect of model enhancements on NO\textsubscript{x} (left) based on tabulated full NO\textsubscript{x} source terms (right). The solid lines refer pdf integrated source (w/ TCI) method, the dotted lines are results from without pdf integrated source (w/ TCI) method. FGM\textsubscript{ph}(in green), FGM\textsubscript{p}(in black).

...tions. This is not necessarily true for FGM\textsubscript{p} as there the \(T_{\text{flamelet}}\) can differ significantly (see Figure 4.18). Similar effects due to FGM model enhancements on NO\textsubscript{x} predictions are observed for both with and without TCI, with slightly higher magnitudes for the latter.

Figure 4.25: Contour plots of CFD temperature, retrieved flamelet temperatures from FGM\textsubscript{ph} and FGM\textsubscript{p} when piston is at 720 °CA.

The above description is only based on a comparison of in-cylinder average quantities. To strengthen the observations, the heat loss effect on the model predictions is visualized. Firstly, the contours of \(T_{\text{CFD}}\) and \(T_{\text{flamelet}}\) from both FGM models are compared in Figure 4.25. It is evident here that the \(T_{\text{flamelet}}\) retrieved from FGM\textsubscript{ph} is in very close match with the \(T_{\text{CFD}}\), while it is higher in case of FGM\textsubscript{p}. Secondly, the contours of \(T_{\text{flamelet}}\) (top) and source terms of pdf integrated NO\textsubscript{x} (bottom) are plotted at two different CA position i.e. 730°CA and 740°CA in Figure 4.26 and 4.27 respectively. These two crank angle positions are chosen due to the higher chances for heat losses. The FGM\textsubscript{p} case is plot-
ted in the left side and $FGM_{ph}$ on the right side of the figures. It can also be seen from the figures that the plume develops downstream, hits the piston lip, and moves towards the cylinder head. Another part moves along the piston bowl. These are the potential locations (as marked with boxes) where the major heat loss occurs from the hot plume to the walls while other regions show moderate heat loss effect. From Figure 4.26, it can be observed that the $FGM_{ph}$ captures heat loss effect by lowering the flame temperatures which, in turn, reduces source terms of $NO_x$ compared to the case with $FGM_p$, at 730°C position. The comparative reduction of source terms (peak values) is by around three times. It is even substantiated more at 740°C position, as shown in Figure 4.27 due to higher heat losses in the vicinity of the piston bowl and cylinder head. Thus, it demonstrates the ability of the higher dimensional FGM with enthalpy as an additional look up variable i.e. $FGM_{ph}$ to take into account of the effect of thermal stratification on the $NO_x$ chemistry evolution.

The trends of these $NO_x$ predictions from tabulated source approach are very well comparable to that of the estimated source approach (see Figure 4.20). Here, for the estimated source approach the $T_{CFD}$ is important only so any difference must be due to the radicals retrieved whereas for the tabulated source approach also the $T_{flamelet}$ is important.

Figure 4.26: Contour plots of retrieved flamelet temperature (top) and source terms of $NO_x$ (bottom) from $FGM_p$ model (left) and $FGM_{ph}$ model (right), when piston is at 730°CA.

4.8 Conclusions

In this chapter, the FGM model enhancements and their impact on combustion characteristics of engine cycle simulations are presented. The methodology is extended to account
for the effect of variable pressure and heat loss on chemistry evolution. Besides, the FGM model with enhanced model settings, such as best table resolution, more detailed n-heptane reaction mechanism for FGM tabulation, and better treatment for evaporative fuel scalar, are incorporated in engine simulation for the first time.

Firstly, a pressure dependent FGM (multiple pressure levels where tables are generated) is applied for both early injection (PCCI) and conventional injection (CDC) timing cases. The main difference in the FGM approach for these two different combustion modes is that Homogeneous Reactors (HR) based FGM database are used for PCCI case, whereas Igniting Counterflow Diffusion Flames (ICDF) based FGM databases are used for CDC case. The Pressure dependent FGM shows notable influence on the ignition delay predictability, for both the injection timing cases. In both cases, the prediction of the ignition delay is accurate and becomes independent of the number of pressure levels at a 5-level table. It should be noted however that for the conventional injection case, where the auto-ignition delay is shorter, a single pressure table at average pressure conditions still provides reasonable results whereas it fails completely for the early timing case. A rapid rise in the heat release rate in both cases is observed, the main reason for this is the inherent short burn duration of the reaction mechanism used. In case of CDC, the discrepancies are observed in the peak cylinder pressure and cumulative heat release (over-prediction) which mainly stems from the differences in the lower calorific value of n-heptane (used in modeling) and that of the real diesel fuel (used in experiment). The single stage ignition from HR resulted in short combustion duration i.e. incomplete combustion by the model, in case of PCCI. This caused an under-prediction of peak cylinder pressure (and cumulative heat release rates).
Further, the FGM model is extended with enthalpy as additional dimension to account for heat loss effect on chemistry evolution. In an a-priori study, the necessary levels of enthalpy are determined from the CFD data. Then, the chemistry database is extended with 5 enthalpy levels at each pressure level. The enhanced FGM model with the extended chemistry database showed a minor impact on global characteristics, such as a lowered initial premix heat release rate. The reason for the observed low impact is the influence of heat loss on the source terms evolution around ignition timing. On the other hand, the Pressure and Enthalpy based FGM model has major influence on the local flame temperature and species spatial distribution during diffusive combustion phase and shows substantial impact on the $NO_x$ predictions. Various approaches to implement $NO_x$ models with FGM framework are used. All are based on a transport equation for $NO$ or $NO_x$ with only difference in the formulation of the source terms.

- In the first approach, the source terms of $NO$ is estimated in terms of either steady state/equilibrium value for the important radicals or direct retrieval of radicals from tables. This study revealed that (i) the steady state approach yields lower $NO$ prediction (approximately 3 to 4 times) due to lower mass fraction of steady state species compared to retrieval approach for both FGM models, (ii) the effect of FGM model enhancements are only significantly evident for Zeldovich detailed approach.

- In the second approach, the source terms of $NO_x$ is directly retrieved from the FGM tables. For these models, it is clearly visualized that the $NO_x$ formation reduces close to the walls (cylinder head/piston) in case of Pressure and Enthalpy dependent FGM when compared to only Pressure dependent FGM. This is due to the ability of Pressure and Enthalpy dependent FGM model to take the heat loss effect while interpolating data from more relevant table when compared to only Pressure dependent FGM model.

Hence, it is demonstrated that the model enhancements with pressure and heat loss dependency on FGM can improve the ignition delay predictions and local flame conditions. Further, as an outlook, capturing the more accurate burn duration is vital for improving the match for global characteristics such as pressure and heat release rates. The table extended for post combustion event can help to perform full simulations with $NO_x$ models, where the results can be validated against the engine-out data directly.
5.1 Introduction

Soot formation in diesel spray combustion is an eminent problem because of the favorable conditions such as high temperature, high pressure, fuel rich conditions due to the liquid spray, and diffusion combustion. The engine-out soot in the form of ultra-fine particulates (generally referred to as particulate matter (PM)) impact human’s health and atmospheric radiation levels adversely. Therefore, stringent emission norms are imposed on engine manufacturers by governance agencies. Apart from that, soot is resultant of incomplete combustion and it leads to high radiative heat losses (about 20-35 % of total heat loss) within the cylinder [Heywood, 1988]. Hence understanding soot formation phenomena in-order to control the net soot production is gaining interest in engine research and development. Figure 5.1 shows the main processes involved in soot formation starting with nucleation from gas phase molecules, particle surface growth, coagulation, agglomeration and simultaneous oxidation processes. The ability to predict soot formation using computer models is one of the key aspects to assist in the optimization of engine performance, now-a-days. However, unlike $NO_x$, the majority of the soot formed will be oxidized which makes the net soot yield more difficult to predict. Since the complex formation and oxidation processes are sensitive to the local flame conditions, the multidimensional modeling of soot processes incorporating a turbulent spray with detailed chemistry becomes even more challenging. The main objective of this work is to devise a simple two equation soot model within the framework of the Flamelet Generated Manifold (FGM) method to predict the diesel soot formation.

![Figure 5.1: Schematic of soot formation and oxidation processes [Bockhorn, 1994].](image_url)
The soot kinetics for this model is obtained from the experience of sectional models [Sirignano et al., 2010 D’Anna et al., 2010 Sirignano et al., 2011], however adopted in the form of a multi-step phenomenological soot model. The model accounts for a nucleation process based on polycyclic aromatic hydrocarbons (PAH), growth, coagulation and oxidation. The reaction mechanism that is used in this study includes PAH (upto two or four rings) which serve as the precursors for the nucleation step. First, the devised soot model is applied to generate the well known $\phi - T$ maps to validate the soot kinetics at various equivalence ratio mixtures ($\phi$) and temperatures (T). This focuses on the soot kinetics and avoids the turbulent flow field effects. The source terms for soot parameters are estimated from the species and temperatures retrieved from the tables. The tables are generated using Homogeneous Reactors. The extensive soot maps that are available in literature [Kitamura et al., 2002] are used to validate the results for soot yield, soot particle number density and soot particle mean diameter. Finally, the model is extended to simulate the soot formation in the ECN Spray H case [ECN, 2012]. Here, the essential requirement for the success of soot modeling is accurate prediction of gas phase chemistry. The best settings for the FGM model coupled to the CFD solver (STAR-CD), obtained from Chapter 3 are applied for turbulent spray combustion in a constant volume combustion chamber. Igniting Counterflow Diffusion Flamelets (ICDF) are used for FGM generation, hence the unsteady effect like ignition is taken into account. The experimental data from Planar Laser Induced Incandescence (PLII) and Laser extinction [Musculus and Pickett, 2005, ECN, 2012] are used to evaluate the model results.

In this chapter, first a brief literature review of the soot models for diesel combustion is presented. Next, the details of the soot kinetics used in the current study are given. Then, the generation of $\phi - T$ and validation with literature data is provided. Further, the soot model implementation for CFD combustion model is presented. Finally, conclusions and an outlook is given.

### 5.2 Soot modeling - Literature review

For the last 5 decades, great progress has been achieved with a variety of soot models ranging from simple to complex. Models can be majorly classified into three categories namely two step empirical, multi-step phenomenological (MSP) and detailed kinetic soot models as shown briefly in Figure 5.2.

The detailed kinetic soot models with sub-mechanisms describing soot particle dynamics along with gas phase chemistry (upto PAH) can predict not only global soot quantities but also the spatial distribution in-terms of particle number density for simple combustion systems. These methods solve a lot of details, mainly in-terms of particle size distribution function (PSDF). The two methods commonly used are either the ‘method of moments’ [Frenklach and Harris, 1987] in which a few moments of the PSDFs are solved, or the ‘sectional method’ [Smooke et al., 2004, D’Anna and Kent, 2003 D’Anna and Kent, 2006] where the particles are subdivided into sections or bins based on sizes of interest and solves equations for them. Although these methods are computationally very expensive, due to the advancements in present modeling techniques and computational power, they have been gaining interest in practical applications [Pitsch et al., 1995 Pitsch et al., 1996 Karlsson et al., 1998]. However, these models are still inconvenient for direct use in
Figure 5.2: A brief view of various soot models ranging from simple to complex.

Routine practical CFD simulations due to many other factors. First, these models require an accurate turbulent combustion model. Acceptable uncertainties in these model predictions (for temperature, species) can even lead to significant deviations in soot predictions. For instance, recent studies of detailed soot modeling using the method of moments for laboratory flames using LES/PDF methods revealed that a relative small inaccuracy in PAH chemistry predictions can lead to a major discrepancy in soot volume fraction predictions [Donde et al., 2013, Mueller and Pitsch, 2012]. Secondly, detailed reaction mechanisms are needed which include PAH, and intermediate species that are of importance for soot sub processes. For engine application, the predictions of these detailed chemical models are influenced to a great extent by the description of the soot model as well as by the sub models for other complex processes such as the turbulence, fuel spray, and species transport. So the main benefits of using a detailed kinetic soot models in practical application might be suppressed due to the uncertainties associated with sub-models for the pre-particle phase [Tao et al., 2005].

On the other hand, the empirical/phenomenological models are based on single or multiple global step reactions describing each sub-process of soot formation. The simplest of all is the 2-step model which is formulated by Hiroyasu after the review of soot models reported from 1962 to 1984 [Hiroyasu et al., 1983]. This model is essentially based on two empirical formulas for predicting the formation and oxidation of soot particles. The soot formation step directly links the concentration of fuel vapor based on high temperature reactions and the oxidation step describes the destruction of soot particles via the attack of molecular oxygen. Although the model [Patterson et al., 1994] gained popularity as it is easily applied in multi-dimensional diesel engine simulations, its applicability range is limited. In many parametric studies with various engine operating conditions, where the low-temperature reaction channels dominate the soot formation processes, the Hiroyasu’s high-temperature soot formation model is not suitable anymore [Liu et al., 2004, Kim et al., 2005, Munnannur et al., 2005].
On the basis of quantitative measurements, Tesner et al., presented a model [Tesner et al., 1971] and postulated a stage of formation of an intermediate species. This species was considered to be responsible for the particle inception/nucleation leading to soot. Thus the direct link between fuel vapor and soot can be relaxed in this model. The model was improved by [Surovikin, 1976] and he showed that the assumption of this intermediate stage could lead to good agreement with experimental data over a wide range of conditions. Consequently, the model is further adopted by various researchers [Zellat et al., 1990; Nishida and Hiroyasu, 1989; Nakakita et al., 1990; Gorokhovski and Borghi, 1993] by including soot inception based on the intermediate species in diesel combustion simulations and achieved acceptable results. Further, Belardini et al., [Belardini et al., 1993; Belardini et al., 1996] postulated this species to be Acetylene, the direct product of a one-step fuel pyrolysis reaction.

In addition to predicting the mass fraction of soot, it is also important to predict the particle number density in diesel combustion process. Hence, few researchers, following the idea of Gilyazetdinov’s work on carbon black formation [Gilyazetdnov, 1972], postulated a mono-disperse size distribution of soot particles and then modeled the soot formation by one or two equations: One for the particle volume fraction and the other for the particle number density. Kennedy et al., [Kennedy et al., 1990] and Moss et al., [Moss et al., 1989] both demonstrated that this approach can give encouraging results. However, due to its limited range of applicability this did not gain much attention. Leung and Lindstedt [Leung et al., 1991; Lindstedt, 1994] used the first two moments in the method of moments, one for volume fraction and the other for particle number density, to calculate soot properties. In their work, they also argued that the intermediate species contributing to the soot particle formation should be connected to at least pyrolysis kinetics of the fuel also used acetylene as intermediate species. In further studies, it has been proposed to use PAH as building blocks or precursors for soot nucleation [Kazakov and Foster, 1998; Viswanathan and Reitz, 2009].

With the aim to construct a generic model framework for diesel soot formation, higher level models with multi global steps were proposed [Fusco et al., 1994; Belardini et al., 1996]. They include global rate expressions for all physical processes like pyrolysis, inception, surface growth, coagulation and oxidation. An 8-step phenomenological soot model [Fusco et al., 1994] is presented where a generic soot precursor radical is proposed for particle inception and specified acetylene as the only species responsible for surface growth. This approach allows the soot formation step to be separated into two reactions with different activation energies, with which both high-temperature and low-temperature formation regimes can possibly be covered. This model is implemented in KIVA-II by solving transport equations for soot volume fraction, soot precursor radicals, acetylene, and particle number density. Hence the model is obviously advantageous because it includes particle dynamics, and is able to predict the mean particle size and the number density of soot particles formed in engines. Due to the fact that inclusion of intermediate steps for soot formation and predictability of soot number density, which is one of the parameters of interests, the MSP modeling approach gained much attention which lead to a continuous improvement in the same framework in the diesel soot modeling community.

This model is further modified by Kazakov et al., [Kazakov and Foster, 1998] with the consideration of higher polyaromatic hydrocarbons (PAH) as precursor species. This new model with 9 steps is implemented in the KIVA-II to model soot in a single cylinder HDDI
diesel engine. The model results compared reasonably well with that of optical in-cylinder soot measurements. The analysis of the soot formation process is also consistent with experimental observations. However the competition between soot precursor and acetylene in these models resulted in some inconsistencies when applied to a wide range of engine conditions. Hence few modification are done by some researchers [Liu et al., 2005 Tao et al., 2009] and lead to a revised multi-step phenomenological soot model. They were applied to model and study the low-temperature soot formation processes [Liu et al., 2005] by varying EGR rates and perform optimization studies with multiple injections for an HSDI diesel engine [Tao et al., 2005]. The results demonstrated that the revised MSP soot model improved the predictions of soot emissions considerably when compared to that of a two-step, basic MSP model. Further to it, to improve the model fidelity a quasi-steady state $H_2-O_2-CO$ system was introduced for $OH$-related soot oxidation [Tao et al., 2009]. This revised 9-step phenomenological soot model is implemented and validated in a wide range of engine conditions with a decent match to the observed trends of soot. This study suggested that these models are fundamentally consistent with the physics and chemistry of soot formation and oxidation processes in diesel engines, are computationally efficient such that they are suitable to be integrated with genetic algorithms for engine system optimization.

In this current work, a similar philosophy as that of other 2-equation models with multi step soot formation is applied however with a slightly different formulation. In the next section, the details of the soot kinetics, used in this work, will be presented.

5.3 Soot kinetics

The soot kinetics used in this work has been derived from a complex multi-sectional model [Sirignano et al., 2010]. In the original scheme, soot is divided into lumped species based on the content in terms of carbon atoms, hydrogen atoms and the state of aggregation (single molecules, single particles and aggregates of particles). The model provides a complete description of the soot properties yet is computationally too demanding to apply in real applications. Hence, most part of these details are not included in the kinetics used here. However, the experience on soot formation modeling in laminar flames [Sirignano et al., 2010, D’Anna et al., 2010 Sirignano et al., 2011] using this detailed model has driven the reduction of the kinetics in a form suitable for the FGM approach.

The kinetics for the basic physical and chemical processes that are considered important for soot formation are: nucleation, growth, coagulation, polymerization and oxidation. These processes are explained shortly in the following.

- Nucleation is the first step that leads to the formation of a soot particle, from the largest gas phase Polycyclic Aromatic Hydrocarbons (PAH) which are referred to as soot precursors. In this work, Naphthalene ($C_{10}H_8$, two ring aromatic $A_2$) is assumed to be the precursor. The nucleation mechanisms considered here comprise both the sticking of two Naphthalenes and the reaction between a Naphthalene and a Naphthyl radical. In both cases the process leads to a compound which is not considered to be in the gas phase anymore and hence is referred to as soot.

- This very first nucleus can undergo a growth process through the addition of acetylene ($C_2H_2$) and other PAH from the gas phase. These processes start with the formation
of a radical on soot species. The radical can be formed through the spontaneous loss of a hydrogen atom from the soot surface or the extraction of a hydrogen atom through the attack of H or OH radicals largely present in the combustion environment. The correct estimation of radical formation rate is crucial for the prediction of the amount of radicals and hence the rate of the subsequent processes such as the surface growth.

- The soot particles produced via nucleation paths can also undergo a coagulation process simultaneously. This process is a physical interaction between two stable particles and no chemical bond is formed. It is generally size dependent and it is modeled balancing the interaction forces (Wan der Waal forces) and the thermal rebound. This means that this process is favored at low temperature and for large particles, which have larger attraction potential. The particles can also form a chemical bond to link each other. This process can be described similarly as a polymerization process, involving a stable and a radical soot particles which form a larger one. Both the coagulation and the polymerization process do not affect the total mass of soot but they change the number concentration and the molar concentration, affecting the final rate of all the other processes.

- Finally, the particles can undergo an oxidation process through the attack of OH if a stable particle is considered or $O_2$ if a radical particle is involved.

All the processes described above result in soot which is characterized here by two quantities, i.e., soot carbon concentration $C_{(s)}$ [mol/cm$^3$] and soot particle number density $N_S$ [#/cm$^3$]. The net rates are,

$$\frac{d(C_{(s)})}{dt} = \omega_{\text{nucleation}} + \omega_{\text{growth}} - \omega_{\text{oxidation}}, \quad (5.1)$$

$$\frac{d(N_S)}{dt} = N_A \left( \frac{\omega_{\text{nucleation}}}{N_c} \right) - \left( \omega_{\text{coagulation}} + \omega_{\text{polymerization}} \right), \quad (5.2)$$

where, $N_A$ is the Avogadro number.

It is possible to derive the mean number of carbon atoms, $N_c$, per soot particles as

$$N_c = \left( \frac{C_{(s)}}{N_S} \right) N_A \quad [-]. \quad (5.3)$$

The global rates for each process is given as below,

$$\omega_{\text{nucleation}} = 20k_{s1}[A_2][A_2^*] + 20k_{s2}[A_2][A_2] \quad [\text{mol/cm}^3\text{s}]$$

$$\omega_{\text{growth}} = 2k_{s8}[\text{Soot}^*][C_2H_2] + 10k_{s9}[\text{Soot}^*][A_2] + 10k_{s10}[\text{Soot}][A_2^2] + 10k_{s11}[\text{Soot}][A_2] \quad [\text{mol/cm}^3\text{s}]$$

$$\omega_{\text{oxidation}} = 2k_{s14}[\text{Soot}^*][O_2] + k_{s15}[\text{Soot}][OH] \quad [\text{mol/cm}^3\text{s}]$$

$$\omega_{\text{polymerization}} = k_{s12}[\text{Soot}][\text{Soot}^*] \quad [\text{mol/cm}^3\text{s}]$$
\[ \omega_{\text{coagulation}} = k_{s13}[\text{Soot}][\text{Soot}] \ [\text{mol/cm}^3\text{s}]. \]

The kinetic parameters for the individual global reactions are reported in Table 1. Note that the soot molar concentration \([\text{Soot}] \ [\text{mol/cm}^3]\) can be derived from the soot particle number density and Avogadro number according to,

\[ [\text{Soot}] = \frac{N_s}{N_A}. \quad (5.4) \]

The concentration of radical \([\text{Soot}^*] \ [\text{mol/cm}^3]\) is calculated with a truncated steady state approximation or taking \(\frac{d[\text{Soot}]}{dt} = 0\), resulting in the following expression:

\[ [\text{Soot}^*] = \frac{[\text{Soot}]}{[H]k_{s4} + [H_2]k_{s6} + [C_2H_2]k_{s8} + [A_2]k_{s9} + [\text{Soot}]k_{s12} + [O_2]k_{s14}}. \quad (5.5) \]
Table 5.1: Reactions and kinetic parameters for soot particles [Sirignano et al., 2010].

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Nucleation</strong></td>
<td></td>
</tr>
<tr>
<td>( A^*_2 + A_2 \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s1} = 1E13 , T^{0.5} \exp(-15000/RT) )</td>
</tr>
<tr>
<td>( A_2 + A_2 \rightleftharpoons \text{Soot} + H^* )</td>
<td>( k_{s2} = 2E15 , T^{-1.5} )</td>
</tr>
<tr>
<td><strong>Radical Initiation</strong></td>
<td></td>
</tr>
<tr>
<td>( \text{Soot} \rightleftharpoons \text{Soot}^* + H )</td>
<td>( k_{s3} = 4E19 , \exp(-113100/RT) )</td>
</tr>
<tr>
<td>( \text{Soot}^* + H \rightleftharpoons \text{Soot} )</td>
<td>( k_{s4} = 8E13 )</td>
</tr>
<tr>
<td>( \text{Soot} + H \rightleftharpoons \text{Soot}^* + H_2 )</td>
<td>( k_{s5} = 1.2E17 , \exp(-16000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot}^* + H_2 \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s6} = 4E7 , \exp(-16000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot} + OH \rightleftharpoons \text{Soot}^* + H_2O )</td>
<td>( k_{s7} = 1.2E16 , \exp(-16000/RT) )</td>
</tr>
<tr>
<td><strong>Growth</strong></td>
<td></td>
</tr>
<tr>
<td>( \text{Soot}^* + C_2H_2 \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s8} = 1E10 , T^{1.87} \exp(-3262/RT) )</td>
</tr>
<tr>
<td>( \text{Soot}^* + A_2 \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s9} = 1E16 , T^{0.5} \exp(-15000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot} + A^*_2 \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s10} = 1E16 , T^{0.5} \exp(-15000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot} + A_2 \rightleftharpoons \text{Soot} )</td>
<td>( k_{s11} = 2E15 , T^{-1.0} )</td>
</tr>
<tr>
<td><strong>Coagulation and Polymerization</strong></td>
<td></td>
</tr>
<tr>
<td>( \text{Soot} + \text{Soot}^* \rightleftharpoons \text{Soot} + H )</td>
<td>( k_{s12} = 2E15 , T^{0.5} \exp(-15000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot} + \text{Soot} \rightleftharpoons \text{Soot} )</td>
<td>( k_{s13} = 2E15 , T^{-0.25} )</td>
</tr>
<tr>
<td><strong>Oxidation</strong></td>
<td></td>
</tr>
<tr>
<td>( \text{Soot}^* + O_2 \rightleftharpoons \text{Soot} + 2CO )</td>
<td>( k_{s14} = 2E15 , \exp(-8000/RT) )</td>
</tr>
<tr>
<td>( \text{Soot} + OH \rightleftharpoons \text{Soot} + HCO )</td>
<td>( k_{s15} = 1E16 , T^{0.5} \exp(-10600/RT) )</td>
</tr>
</tbody>
</table>

Units are in \( \text{mol} \), \( \text{cal} \), \( \text{cm} \), \( \text{s} \), \( \text{K} \).
5.4 $\phi$ - $T$ maps

Soot $\phi - T$ maps are widely used as simple indicative diagrams to show the soot formation tendencies for various mixtures. In this section, these maps are generated using the newly devised 2-equation based soot model using an FGM-like approach and validated against the published data. First, the model setup used for $\phi - T$ generation is described and then the validation results are presented.

5.4.1 Model setup

![Flowchart of the model for $\phi - T$ maps generation, at a given condition of $\phi$ and $T$.](image)

Figure 5.3: Flowchart of the model for $\phi - T$ maps generation, at a given condition of $\phi$ and $T$.

Figure 5.3 shows the flowchart of the model setup. To mimic FGM-like approach, the chemistry database is tabulated a-priori and coupled to online calculations. So, the first step in this approach is preprocessing of the database. Homogeneous Reactor (HR) (see Section 2.3.1) calculations are performed at various initial mixture conditions of different equivalence ratios ($\phi$), at different temperatures ($T$). To be consistent with the conditions used in the generation of $\phi - T$ maps in literature, the HR database is generated using iso-thermal conditions while maintaining a constant pressure of 60 bar. The oxidizer is pure air (i.e. 21% $O_2$ and 79% $N_2$) and the fuel is $n$-heptane. The reaction mechanism used is a combination of the Andrae mechanism for $n$-heptane oxidation and the $NO_x$ mechanism of GRI 3.0 (the same as the one used in engine cycle simulations in Section 4.2.3 in Chapter 4) including a PAH ($A_1$-$A_4$) mechanism [Skjøth-Rasmussen et al., 2004]. The total mechanism includes 1011 reactions amongst 229 species. The raw data generated in temporal space at different values of $\phi$ are transformed into mixture fraction ($Z$) and progress variable ($\gamma$) co-ordinates, at each temperature condition. Hence the table will have three dimensions being $T$, $\phi$ or $Z$ and $t$ or $\gamma$. For all $\phi$, $T$ combinations in the map, soot and
number density are computed. The source terms are computed using the retrieved species mass fractions from pre-tabulated detailed gas phase chemistry. Note that the consumption of the gas phase carbon due to soot formation is not taken into account. Subsequently, soot yield and mean particle diameter (assuming spherical particles) are derived using the following expressions:

\[
\text{Soot yield} = \left( \frac{C_s}{7 \left[ C_7H_{16}\right]_{\text{(init)}}} \right) 100, \tag{5.6}
\]

\[
d_p = \left( \frac{6 m_c C_s}{\pi \rho_{\text{soot}} N_s} \right)^{1/3}, \tag{5.7}
\]

where \( [C_7H_{16}]_{\text{(init)}} \) is the initial fuel vapor concentration (mol/cm\(^3\)) at each \( \phi - T \) condition, \( m_c \) is the molecular mass of carbon, and \( \rho_{\text{soot}} \) is soot density (assumed to be 2.0 g/cm\(^3\)).

### 5.4.2 Results: \( \phi - T \) maps validation

Now, the generated \( \phi - T \) maps are compared with the published \( \phi - T \) maps. These published maps are generated by Kitamura et al [Kitamura et al., 2002]. In that work, the soot kinetics model is based on a more detailed description of PSDFs using the method of moments and a direct coupling with the homogeneous gas phase chemical kinetics (CHEMKIN/SENKIN) code. So unlike the current model, they couple the soot chemistry directly to the hydrocarbon gas phase chemistry. The nucleation starts from a precursor with 7 ring PAH (i.e., coronene) and is based on the modified Smoluchowski model [Smoluchowski, 1917], surface growth is by the modified HACA (Hydrogen Abstraction Carbon Addition) model [Frenklach and Wang, 1990] and the oxidation by molecular oxygen and OH radicals. The model is validated against shock-tube experiments by Kellerer et al., [Kellerer et al., 2000]. More details of this work can be found in [Kitamura et al., 2002].

As a first step, the gas phase chemistry model is validated comparing the key gas phase species. Data for acetylene \( (C_2H_2) \) and benzene \( (C_6H_6) \) is available in the published work. These species are considered to be very important as acetylene influences the soot particle growth while benzene being a single ring aromatic is responsible for the further growth of PAH and soot particle formation. Hence, both species are compared for the current model and the published data are shown in Figure 5.4. The current gas phase chemistry model which is based on the FGM-like tabulated approach, captures the main structure of these species profiles in \( \phi - T \) space. Both quantitative and qualitative agreement is obtained in many regions (at least at relatively low temperatures). In case of acetylene, at high temperature (\( \geq 1900 \) K) and high equivalence ratio (\( \geq 4 \)) conditions, our model over-predicts the concentration considerably when compared to that of the published maps. In the case of benzene, the peak region is slightly shifted to higher temperatures. This discrepancy is consistent with the differences observed at high temperature conditions by Rasmussen et al., [Skjøth-Rasmussen et al., 2004] who developed the aromatic chemistry model. However, the model is in good agreement in the main regions where the soot formation typically is high.
Further, the maps for soot quantities obtained from the current model are compared with results found in published work (Figure 5.5). The plots on the left are the published data, and on the right are the model output. The following observations are made:

- Soot yield [%] is plotted in the range of T (1000K -3000 K) and $\phi$ (0-7), in the top plot of Figure 5.5. The two main observations of the reference soot yield maps are (1) the well-known bell-shaped temperature dependence for a fixed equivalence ratio, (2) a slight shift in peak soot formation towards higher temperature as equivalence ratio increases. The simplified soot kinetics applied in the FGM-like detailed chemistry model very well capture these tendencies in soot production. The magnitudes show a very good match. Only deviation is observed for the location of peak regions, which could stem from the differences in aromatic species used as the initiators for soot nucleation.

- Next, the soot particle number density ($N_S$) [#/$cm^3$] is mapped in the middle plot of Figure 5.5. It is observed from the published maps that high concentrations of particles are found in the temperature range of 1400 K - 1800 K. The peak values of particle number density move towards lower temperatures as equivalence ratio in-
creases. This is due to the fact that the coagulation rates reduce at these low temperature regions, where the particle collisions diminish. Thus, the soot content and particle formation is mainly characterized by the shift in the peninsula of particle number density from that of the soot yield. The maps from the current model shows a similar behavior. However, the published maps show a more drastic reduction in the particle number density while moving away from the region of 1400 K - 1800 K,
whereas the maps from the model show a more gradual reduction in particle number density. This is because in the current model coagulation and polymerization are less sensitive to a change in temperature which influences the net soot particle numbers.

- The maps of particle mean diameter ($d_p$) [nm] are compared in the bottom plot of Figure 5.5. The model captures the trend of having bigger particles at high temperatures and equivalence ratios. As expected, this is completely opposite to the trend for the particle number density. However, the published map depicts a bell-shaped temperature dependence for particle size mainly at high equivalence ratios. The current model shows a deviation with this observation, due to the discrepancy found in the maps of particle number density in the same regions. Note that the particle size is a derived quantity (using equation 5.4.1) from soot concentration and particle number density.

From the above observations, it can be concluded that the simple two equation based soot model is able to reproduce the soot tendencies, mainly the $\phi-T$ regions of importance. These regions include the conditions similar to that found in conventional diesel combustion where the high soot production occurs.

## 5.5 CFD modeling

In this section, the soot model is integrated in the 3D CFD simulation for dedicated sprays of $n$-heptane (i.e. Spray H). The availability of experimental soot data from the ECN database is one of the main motivations for this work. Here, first the soot model implementation is briefly introduced and then a systematic analysis of the results is presented.

### 5.5.1 Model setup

The 2-equation based soot model is implemented in the same CFD-FGM framework, as explained in Chapter 3. The integration of soot model is shown in the schematic in Figure 5.6. It can also be visualized as an extension of the model for $\phi-T$ maps. Instead of MATLAB, STAR-CD is used to resolve the spray, mixing and flow field. The same sub-models for spray and turbulence that are used in Chapter 3 are applied here. Note that the radiation heat loss effect is neglected. The pre-tabulation of the chemistry database (FGM table) here is performed based on the ICDF configuration, instead of the HR which was used for the $\phi-T$ maps. More details of the ICDF model can be found in Section 2.3.1 of Chapter 2. The same detailed reaction mechanism along with PAH chemistry described in $\phi-T$ maps generation is used here. 101 points in each direction of mixture fraction and progress variable, with quadratic spacing in the progress variable dimension is applied. The source terms for soot quantities are estimated, via a user defined function, based on the retrieved information from the ICDF based FGM tables (in soot kinetics part of Figure 5.6). These net rates are estimated by applying a simple $\delta$-pdf or a well-mixed approach (which mean, $\tilde{\omega} = f(\tilde{Y_i}, T) \neq f(\tilde{Y_i}, \tilde{T})$, for that reason the net rates needed to be re-calibrated.

Soot formation and oxidation are complex processes involving a wide range of heterogeneous processes, hence the CFD soot model’s validation is a challenging task. As an a-priori analysis, first the conditions obtained from typical CFD simulations are projected
on the already constructed soot $\phi - T$ maps (as discussed in earlier section). Then, the ability of the model to capture the phenomenology of soot formation processes is tested. This is done by comparing the model output with the conceptual model developed by Kosaka et al., based on many experimental laser studies [Kosaka et al., 1995, Kosaka et al., 1996, Kosaka et al., 2005]. This exercise is to compare the spatial locations of various species concentrations outputs from the CFD model with respect to the soot in the diesel spray flame. Finally, the model results are validated against the experimental observations from the ECN database. These three analyses are presented here.

### 5.5.2 Projection of CFD ($\phi, T$) data on pre-generated soot maps

Figure 5.7 shows the projection of $\phi, T$ conditions from CFD simulation on soot maps, at various time instances after start of injection. The CFD data shown in colored dots are extracted from the simulation of the baseline Spray H case where the applied ambient conditions are $[O_2] = 21\%$, $T_{ox} = 1000$ K, $P = 42.1$ bar. The contours of soot volume fraction ($f_v$) [ppm] obtained from the soot maps are shown in gray maps. Note here that these soot maps are generated at 42.1 bar, different from the maps used in the previous section which are generated at 60.0 bar conditions. It can be observed from the plots that the CFD data points spread towards high temperature due to the rise in temperature caused by the ignition. The equivalence ratio from CFD is limited to values up to 3. This is due to the low computational cell resolution. The CFD data points which move into the soot peninsula at time instances beyond 1.2 ms are responsible for the net soot formation. The typical favorable conditions for the soot formation i.e., rich mixtures with moderately high temperatures can be identified from these projected regions. This mapping of $\phi, T$ conditions (from a combustion model) on the pre-generated soot maps (based on homogeneous conditions) is often used in the engine research community to identify the sooting regions [Akihama et al., 2011, Kaario...
et al., 2005]. For example in the study of Akihama et al., these projection based maps are used to obtain the mechanisms for smokeless diesel combustion.

### 5.5.3 Validation: Phenomenology of soot formation

So far the $\phi - T$ maps are used to evaluate the soot model performance. Now, the results from the soot model integrated in CFD are evaluated directly to see how good the model captures the total phenomenology of soot formation and oxidation. Kosaka et al., in their work, took simultaneous imaging of soot precursors, OH and particles using Laser Induced Incandescence (LII) and Laser Induced Fluorescence (LIF) experimental techniques in a Rapid Compression Machine to derive a conceptual model for complex diesel soot formation processes. The extended details of this work can be found in [Kosaka et al., 2005]. The conceptual diagram of spray and soot formation processes is shown on the left hand side of Figure 5.8. The schematic depicts the entire structure of sub-processes starting with the spray, the flame, soot formation and soot oxidation processes (also refer Figure 5.1) in a typical quasi-steady transient flame at 2.5 ms from the start of injection (ASI). On the right side of Figure 5.8, a set of contours obtained from the CFD model for the mixture fraction field, mass fractions of $A_2$, $OH$, soot volume fraction ($f_v$) and soot number density ($N_S$) are plotted from left to right, respectively. All these contours are captured at 3 ms after the start of injection. This gives an excellent opportunity to locate the responsible parameters of interest for the spray, the flame and soot formation and oxidation. The model results can be evaluated with this conceptual model by comparing the following phenomena:

- The conceptual model suggests that, for typical conventional diesel spray conditions, soot precursors are observed in the central core. The precursors on the periphery
nucleate to soot particles of small size, and with high number density. Here, the FGM based combustion model is able to predict this location of precursors in terms of the naphthalene ($A_2$) concentrations, while the applied soot model captures the nucleation to young soot particles as the location of the peak particle number density is in very good agreement with that found in the conceptual model.

- Further, it is indicated in the conceptual model that due to the momentum induced by the spray, these particles move further downstream and experience surface growth and coagulation and become larger particles. Hence the soot concentration at the central core downstream is high. In the current model output, the relative location of peak soot volume fraction ($f_v$) matches with that in the conceptual model.

- Finally, the conceptual model reveals that the soot particles are pushed away from the centerline due to head-vertex motion and after entering to the flame again they get oxidized due to the high availability of $OH$ concentrations in the hot flame. The $OH$ mass fraction obtained from the model shows that $OH$ surrounds the rich flame zone, and hence the soot in that zone gets oxidized and consequentially the region appears to have low soot concentrations.

The normalized source terms for nucleation, growth, coagulation and oxidation, which are shown in Figure 5.9, corroborates the above explanations. The high nucleation rates are close to the tip of the $A_2$ precursors, while the high rates of growth and coagulations...
are observed at slightly downstream locations. The oxidation rates are high in the regions away from the center line, where the $OH$ is high. Hence it can be concluded that the model is able to predict the soot formation and oxidation processes on a qualitative and phenomenological basis. However, the rates of production and oxidation are high so the net soot formation is highly sensitive with the details. The competition between these processes is quite crucial to achieve quantitative agreement with net soot quantities. Hence, in next section, experimental data are used to compare the model predictions.

**Figure 5.9**: Phenomenological validation: Normalized source terms of (from left to right) nucleation, surface growth, coagulation & polymerization and oxidation, respectively.

### 5.5.4 Validation: ECN experimental data

Detailed experiments were performed with in the ECN network to measure the temporal and spatial distribution of soot quantities. In order to capture the time resolved soot at different specified axial locations, line-of-sight extinction (KL) data are obtained in time from the start of injection. Here, $K$ is the extinction coefficient and $L$ is the length of soot path. The soot volume fraction ($f_v$) is estimated using $KL = \int f_v k_e/\lambda \, dz$, where $k_e$ is the optical extinction coefficient, $\lambda$ the wavelength and $z$ the direction of the laser path. Then, a set of 2D images are taken using PLII measurements at different time steps. By integrating these laser extinction data and PLII images, the spatial soot distributions are extracted.

First, the temporal soot volume fraction ($f_v$) evolution from the model predictions are compared with the time resolved KL data from experiments, for the baseline Spray H case. Three axial planes are selected, one being at a location where the peak quantities are
observed and others are 5 mm away on either side. The data from experiments and model are plotted in the left and right of Figure 5.10, respectively. At these locations, a rapid rise in KL values occurs at around 1ms ASI which is due to the arrival of the fuel jet head with substantial soot content. Further, the KL values reduce and fluctuate about a mean value due to the variations in the soot levels in the extinction measurement location with respect to time. The model picks the initial transient phase of soot formation very accurately at the corresponding locations. The quasi-steady nature of soot after the rise is also reproduced by the model. Based on the observation of the quasi-steady nature of soot, the time-averaged KL data (or \( f_v \)) is estimated at each position in a defined time-averaging window. This helped in obtaining the spatial distribution of soot volume fraction, using the 2D images obtained from PLII. This allowed to reduce huge experimental data (transient and spatial changes) set into a single and representative image which can be used for model validation. Hence, in the next step of validation, these spatial distribution images are used for model validation.

The model is extended to simulate the soot in Spray H cases with varying the \( O_2 \) concentrations i.e. 15% and 12% \( O_2 \), in addition to 21% which is the baseline case. The time-averaged contours of soot volume fraction obtained from simulations are compared with those obtained from PLII + Laser extinction experiments (as explained earlier), in Figure 5.11. Note that the time-averaging windows are slightly different for different \( O_2 \) concentrations which are also given in the figure. The liftoff lengths (LOL) are also marked which are based on steady \( OH \) fields. It is observed from the experiments that the maxima of the soot concentrations reduce and the soot region shifts downstream when the \([O_2]\) in the combustion chamber is lowered. The model is able to capture these trends, qualitatively. The LOL and axial location of maximum mean \( f_v \) are compared between experiments and model prediction in Figure 5.12 (left), for all \( O_2 \) conditions. The values of maximum mean \( f_v \) is plotted in Figure 5.12 (right). A deviation occurs in the quantitative values, mainly
Figure 5.11: Variation in the spatial distribution of quasi-steady soot volume fraction ($f_v$) for several values of $O_2$ concentrations in the combustion chamber. (left) ECN Experimental observations, (right) Predictions from current soot model.

showing a different sensitivity to a $[O_2]$ change than for experimental observations. The main suspects for the differences in the soot levels could be the differences in the aromatic levels in the rich mixtures (as described in $\phi - T$ section) and the calibration of the rates due to TCI closure. Moreover, the model under-predicts the location of peak soot, particularly at lower $O_2$ concentrations despite the slight over-prediction of the liftoff lengths. The net soot formation is a results from the competition between the formation, growth and oxidation. It is observed for the low $[O_2]$ cases, the oxidation rates are high at the farthest downstream centerline location (unlike the locations away from the centerline as shown in the phenomenology) hence the peak soot formation is observed in more upstream locations compared to the experiment. It has to be noted that the rates are highly sensitive to locally resolved conditions. Any deviation in $OH$ concentrations and temperatures can affect the results drastically. Further studies have to be carried out to understand this discrepancy with the model at various other conditions, and also more importantly in relation to direct TCI closures. Still, the 2-equation based soot model is able to pick up the qualitative trends due to change in $[O_2]$ levels, i.e. change in EGR levels.

5.6 Concluding remarks

To conclude, in this chapter, the FGM model is extended with a newly devised soot model to simulate the diesel soot formation. The detailed soot kinetic processes are incorporated using a 2-equation model setup in the tabulated chemistry approach which is described in detail. It is found that the soot model with HR based FGM table is able to reproduce the well-known $\phi - T$ maps. Soot model application in the FGM-like approach is simple and computationally less expensive. The model shows a very good agreement with published maps, mainly in the key high soot concentration zones, with a slight deviation found in other zones where the particle number density (and particle size) differs consistently. Further, the model is extended to simulate soot in Spray H cases. The soot model coupled to FGM-CFD
interactions captures the phenomenology (or the relative locations) of soot formation and oxidation after the spray and flame development. It can be concluded that the FGM approach is able to characterize the sub-processes of soot formation and oxidation, qualitatively. The detailed experiment (temporal and spatial) observations from the ECN database are used to evaluate the model predictions. The transient nature of soot jet propagation is well captured by the model for baseline Spray H case. The spatial distribution of soot volume fraction is also qualitatively in good agreement between experiments and model predictions. The sensitivity due to the change in $[O_2]$ in the chamber on the location and magnitudes of peak soot volume fraction is captured by the model. However, a deviation in the quantitative comparison occurs due to the differences in the competition between the relative processes. Better treatment of turbulent chemistry interactions, and testing the model at different operating conditions can help to understand the model behavior further. However, the ideal way of incorporating soot kinetics in FGM is by directly adding it to the reaction mechanism and tabulate the rates, which can be retrieved directly during FGM-CFD interactions. This allows to apply a TCI closure in a better way as well. Nevertheless, it is important to note that the first ever implementation of a simplified soot model in the FGM framework as a model enhancement is successful. The soot model with FGM including detailed chemistry showed very encouraging results by capturing the complex phenomenon of soot formation and oxidation.

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**Figure 5.12:** (left) Comparison of liftoff length (LOL) and maximum mean $f_v$ locations (XMAX) vs $O_2$ change between experiments and model predictions, (right) Peak $f_v$ vs $[O_2]$ for experiments and model predictions.
Conclusion

In this thesis, the application of the FGM model for diesel engine combustion is analyzed and improved. The first ever implementation of FGM for diesel spray combustion modeling already showed its potential, however leaving a huge scope for further improvements still needed to let it become a robust and complete model for diesel engine combustion and emission processes. Hence, the current research work consists of three focal areas aimed at

1. Improving the predictability of FGM for igniting diesel sprays,
2. Accounting for variations in pressure and (mainly) heat losses on the FGM chemistry in engine cycle simulations,
3. Including complex soot kinetics in the FGM framework.

In this chapter, first the key advancements and conclusions are presented and then the recommendations are given as future directions to reach a complete and robust model.

6.1 Advancements

Igniting sprays have its paramount importance in diesel combustion and emission formation, hence modeling this phenomenon as accurately as possible is a very essential task. The modeling of igniting diesel sprays includes main challenges in resolving turbulent spray formation and most importantly, the ignition process. In the current framework, the FGM chemistry (to model ignition) is coupled to the CFD solver (STAR-CD to model turbulent spray formation). Detailed investigations are carried-out to refine the method and to improve the predictability of ignition characteristics. An extensive and unambiguous set of experimental dataset from the Engine Combustion Network (ECN) is used for model validation. These experiments are performed in a constant volume chamber mimicking various 'engine like' conditions with two different diesel surrogate fuels i.e. n-heptane and n-dodecane. Firstly, the most suitable sub-models from STAR-CD that are available for modeling turbulence, spray and mixing are assessed along with model set-up parameters (cell and time step size). From this study, the best combination of settings is obtained to capture a good match with the non-reacting spray characteristics (i.e. liquid and spray penetration) and mixture fraction profiles from experiments. Moreover, the model with the best settings shows a consistent match with experimental spray data for both surrogate fuels. Secondly, the FGM model is coupled (via mixture fraction and progress variable) to STAR-CD to model the
igniting spray and model refinements are studied. The main features of FGM are the selection of the appropriate configurations for database generation, the adequate table resolution and the treatment of turbulent chemistry closure. A detailed approach is used to understand the effects of these features on ignition so as to improve its predictability. In this work, two different canonical configurations are used i.e. Igniting Counter-flow Diffusion Flames (ICDF) and Homogeneous Reactors (HR) which are suitable to account ignition in the FGM tabulation. The main difference between the two tabulation methods is the effect of diffusion and transport during chemistry generation which is only accounted for with ICDF. The FGM table resolution study in both laminar and CFD cases proved that a quadratic spacing in progress variable is important. Using 101 points in each direction is then adequate. The refined resolution of FGM table improved the FGM’s predictability for ignition delay, both quantitatively and qualitatively, for varying $O_2$ conditions of Spray H ($n$-heptane fuel).

Further, the influence of accounting TCI (in FGM tabulation by adding mixture fraction variance) on ignition characteristics is studied. It showed that the effect of the closure on ignition is insignificant and LOL distance is shortened due to the broader distribution of OH in the CFD simulations. Importantly, the inclusion of TCI improved the LOL trends, mainly for the case with ICDF based FGM tables. Progressively, the validation of this enhanced FGM model against a huge parametric sweep of Spray A (i.e. with $n$-dodecane fuel) conditions from the ECN database concluded that, in principle, the FGM method is in very good agreement with the ignition characteristics from experiments. ICDF captures sensitivities for both ignition timing and LOL very well at various conditions, whereas HR is insensitive in capturing the trends for LOL. The low temperature conditions revealed that the methodology of generation needs refinement due to the increased sensitivity of the ICDF’s to straining at these temperatures. The selected strain rate of 500 s$^{-1}$, which is commonly used for ICDF generation, appeared to be too high (near to the ignition limit). This resulted in highly over-prediction of ignition delay. FGM database generated at reduced strain rates improved the ignition predictions. However the flame liftoff lengths was affected adversely.

For engine simulations the FGM approach needs to incorporate the effect of changing pressure and the occurrence of heat-loss, both not present in the Spray H and A studies. The implementation of only pressure dependent FGM at two different operating modes i.e. conventional injection timing (CDC) and PCCI condition revealed that a moderate number of pressures (at least 5) is necessary to capture the start of combustion (SOC) accurately, mainly at PCCI conditions where it is more demanding due to its long separation between injection and ignition. ICDF and HR based FGMs are used for CDC and PCCI respectively. However the short-burn duration characteristics of the mechanism resulted in rapid rise in heat release rates. Moreover, the single stage nature of HR caused incomplete combustion in the PCCI case resulting in under-prediction of peak cylinder pressure. However, the model shows a good match with the SOC from experiments. Subsequently, the pressure dependent FGM model is further extended with enthalpy as additional dimension to account for the heat loss effects on chemistry evolution in CDC case. The pressure and enthalpy dependent FGM shows a minor improvement in the global characteristics like SOC and cylinder pressures. However the impact is significant on predictions of local temperature
and species concentrations due to the cooling effect by walls. Consequently, the pressure and enthalpy dependent FGM showed a major influence on the NOx predictions which are a strong function of local conditions.

Finally, a soot model incorporating detailed sub-processes such as nucleation, growth, coagulation and oxidation is included in FGM for the first time. The modeling of these soot formation and oxidation processes is complex and highly dependent on the accuracy of spray and gas phase chemistry predictions. The newly devised multi-step soot kinetics is first evaluated by generating and validating against published $\phi - T$ maps from literature, where the model showed a good agreement in key regions. Then, the 2-equation based soot model is coupled to the CFD simulation of the Spray H case, of which the reacting spray characteristics are in good agreement with experiments already. The fundamental phenomenology of soot formation and oxidation is well captured by the model. With the validation of the model results against experimental data from ECN, it is concluded that the model based on the 'well mixed approximation' predicts the transient nature of soot formation from the diesel spray and captures the sensitivity of the change in ambient $O_2$ concentrations on soot formation qualitatively.

To conclude, the advances in the FGM approach in the current thesis definitely would bridge the gap from a first ever application to a robust and complete model for diesel engine combustion and emission modeling.

### 6.2 Recommendations

Diesel engine combustion and emission formation is a vast field and modeling such processes is a very demanding task. The reported advances in the FGM application address this task to a large extent. However, a few aspects are still to be investigated. Some recommendations are given here.

Firstly, the success of tabulation chemistry methods depends on the accuracy of reaction mechanisms over a wide range of application. It is recommended to evaluate the FGM model with more improved reaction mechanisms. For instance, a detailed reaction mechanism for $n$-heptane with better burn duration predictability is to be applied in engine cycle simulations to evaluate the improvements with rapid rise in heat release rates. For $n$-dodecane which is a new fuel, a more detailed reaction mechanism which is well validated in the NTC (Negative Temperature Coefficient) regions should be applied and check the improvements with FGM performance, especially at low-temperature combustion (Spray A) conditions. FGM being a tabulated approach is able to handle detailed mechanisms. It is also worthwhile to study the effects of additional dimensions such as variance of progress variable for better treatment of fluctuations due to turbulence, and strain rate (or a third progress variable dimension, $HO_2$ mass fraction) to account for the subtle sense of chemistry due to flow straining. Purely non-premixed (ICDF) or pure homogeneous mixture (HR) tabulation methods are evaluated. However, it is also recommended to test cases (mainly low-temperature combustion) using partially premixed flames. Much detailed experimental data of species might help in the assessment of liftoff length locations.

In this work, pressure and enthalpy variables are added as dimensions in FGM which demonstrated its ability to capture the changes in pressure and heat loss on the chemical source terms. However, the a-priori estimation process of finding adequate levels can be
time-consuming task. Hence it is recommended to use dependency functions, which provide the dependence of changes in pressure and enthalpy (or even enthalpy defect) on chemical source terms, instead of interpolating the quantities from the databases. Careful treatment is needed for post combustion events as the mixture and burning conditions change drastically. This is important to predict emissions accurately.

The soot model used in this thesis has to undergo further improvements and validations at different conditions (from ECN) before using it for engine cycle simulations. Recommendations for further improvements are using higher ring PAH as precursor, a better TCI for the source terms, mainly incorporating soot kinetics in the table generation directly and tabulate the source terms.
Nomenclature

Acronyms

aTDC  After Top Dead Center
ASI   After Start of Injection
CDC   Classical Diesel Combustion
CFD   Computational Fluid Dynamics
CMC   Conditional Momentum Closure
CSP   Computational Singular Perturbation
CTC   Characteristic Time Combustion
DNS   Direct Numerical Simulation
EBU   Eddy Breakup Model
EDM   Eddy Dissipation Model
ECN   Engine Combustion Network
EGR   Exhaust Gas Recirculation
EOI   End of Injection
FGM   Flamelet Generated Manifold
$FGM_p$ Pressure dependent FGM
$FGM_{ph}$ Pressure and Enthalpy dependent FGM
HCCI  Homogeneous Charge Compression Ignition
HDDI  Heavy Duty Direct Injection
HF    Hsiang and Faeth
HR    Homogeneous Reactors
HRR   Heat Release Rate
ICDF  Igniting Counterflow Diffusion Flamelets
ID    Ignition Delay
ILDM  Intrinsic Low-Dimensional Manifold
IVC   Intake Valve Closing
LES   Large Eddy Simulations
LL    Liquid penetration length
LOL   Lift-Off Length
LIF   Lase Induced Fluorescence
LTC   Low Temperature Combustion
MSP   Multi-Step Phenomenological model
MPI   Max Planck Institute
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>MPI2</td>
<td>Modified MPI</td>
</tr>
<tr>
<td>NTC</td>
<td>Negative Temperature Coefficient</td>
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<tr>
<td>PAH</td>
<td>Polycyclic Aromatic Hydrocarbons</td>
</tr>
<tr>
<td>PCCI</td>
<td>Premixed Charge Compression Ignition</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Density Function</td>
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<tr>
<td>PE</td>
<td>Pilch and Erdman</td>
</tr>
<tr>
<td>PLII</td>
<td>Planar Laser Induced Incandescence</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate Matter</td>
</tr>
<tr>
<td>PSDF</td>
<td>Particle Size Distribution Function</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds Averaged Navier Stokes</td>
</tr>
<tr>
<td>RD</td>
<td>Reitz and Diwakar</td>
</tr>
<tr>
<td>RIF</td>
<td>Representative Interactive Flamelet</td>
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<tr>
<td>SGS</td>
<td>Sub-Grid Scale</td>
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<tr>
<td>SL</td>
<td>Spray penetration length</td>
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<td>Start of Combustion</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of Injection</td>
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<td>$T_{CFD}$</td>
<td>CFD gas Temperature</td>
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<tr>
<td>$T_\text{flamelet}$</td>
<td>Flamelet Temperature</td>
</tr>
<tr>
<td>TIF</td>
<td>Transient Interactive Flamelet</td>
</tr>
<tr>
<td>TFPV</td>
<td>Transient Flamelet Progress Variable</td>
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A-priori study on treatment of evaporative fuel scalar

In diesel spray combustion modeling using tabulated chemistry approach, the treatment of evaporative fuel ($C_7H_{16}$) scalar plays an important role in mixture properties calculations which in-turn influence the evaporation rates of newly introduced droplets. And, also it effects the mixture enthalpy (hence temperature) calculations. In this a-priori study, the fuel scalar is treated more appropriately and the impact is studied with improved model for CDC case, using average FGM table.

![Figure A.1](image.png)

**Figure A.1:** Z Treatment of evaporative $C_7H_{16}$ scalar in FGM and STAR-CD coupling. (left) The previous model. (right) The improved model.

The first implementation of FGM (coupling to STAR-CD solver) for engine simulations is carried out with the approach as shown in Figure A.1 (left). The source term (sFU) obtained from the evaporative spray droplets is used to transport the evaporative scalar of $C_7H_{16}$ (i.e. $Y_{C_7H_{16}}$) and mixture fraction term. The reactive scalar of $C_7H_{16}$ (i.e. $Y_{C_7H_{16,table}}$) is interpolated from the FGM table, and is set as active scalar in STAR-CD which will be used to calculate the mixture properties. This influences the evaporation rate using the following expression,
\[
\frac{dm_d}{dt} = -2\pi \frac{k}{c_p} D_d (1 + 0.23 Re^{1/2}) \ln \left[ 1 + \frac{c_p(T - T_d)}{h_{fg}} \right]
\]

Where, \( k \) is the conductivity, and \( c_p \) the specific heat of the mixture. In current approach, this evaporative \( C_7H_{16} \) scalar is treated differently as shown in Figure A.1(right). Firstly, this scalar is extended with reactive sink term (\( sC_7H_{16} \)) which is interpolated reactive source term obtained from FGM tables) in addition to the evaporative source term (\( sFU \)) from spray model. Secondly, this evaporative \( C_7H_{16} \) scalar is made active scalar in STAR-CD for property calculations hence it influences the evaporation rate. In short, there is only one scalar for \( C_7H_{16} \) which is transported and active for mixture property calculations which is more appropriate.

**Figure A.2:** Effect of treatment of evaporative \( C_7H_{16} \) scalar (improved model) and \( C_7H_{16} \) table scalar (previous model) on evaporation rates.

In Figure A.2 the mass fraction of \( C_7H_{16} \) scalar (left) and evaporation rates (right) are compared for two different model setups. The reactive sink term included \( C_7H_{16} \) scalar (in green) shows the consumed portion when compared to that from previous model (in blue). However, the impact on evaporation rates is nominal due to the fact that typically droplets evaporate at much shorter distance compared to the location where ignition takes place. However, the implication of the model enhancement on enthalpy calculation is significant. Figure A.3(left) shows enthalpy vs. \( Z \), and Figure A.3(right) shows the temperature vs. \( Z \) comparison for both model setups and with 1D flames data. The enthalpy and temperature predictions from improved model setup are comparable with that from 1D flames data which is expected, whereas the plot from previous model setup deviates. In previous model setup, the presence of fuel vapor (for instance, extending the blue dots until the \( Z=1 \) (fuel) will never meet the expected values of enthalpy or temperature) does not felt in the enthalpy calculations which leads to relatively higher enthalpy which results to higher temperatures.

In Figure A.4, the contours of temperatures when piston at TDC shows the impact of the model enhancement. The improved model shows lower temperatures particularly at rich flame side. Then, the global engine combustion characteristics such as pressure
Figure A.3: Scatter plot of Enthalpy (left) and Temperature (right) versus Mixture Fraction for improved model (green), previous model (blue)- when piston at TDC; and, compared with 1D counter flow steady flames at three different pressures (red).

Figure A.4: Contour plots of Temperature for improved model (left) and previous model (right), when piston at TDC.

trace and heat release rate trace are compared in Figure A.5. The improved model shows a great impact by reducing the peak values (around 5% in pressure, and 18% for HRR) and achieves better match with experimental data, although there is no effect on the ignition delay predictions. This simulations are with average FGM table.

Hence, based on this study, it is revealed that the appropriate treatment of $C_7H_{16}$ scalar affects the evaporation rates marginally however it has an significant effect on enthalpy (and temperature) calculations. And, in turn, it improves the cylinder pressure (and heat release rates) trace. So the improved model setup is used during further studies.
Figure A.5: Cylinder pressure trace and heat release rate (HRR) trace for CDC. Experimental data (blue), previous model (red) and improved model (green).
Appendix B

NO model

Extended Zeldovich mechanism:

\[
\begin{align*}
NO + N & \underset{k_1}{\overset{k_{-1}}{\rightleftharpoons}} O + N_2 \\
N + O_2 & \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} NO + O \\
N + OH & \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} NO + H
\end{align*}
\]

The reaction rate constants are expressed as,

\[
\begin{align*}
k_1 &= 7.6e^{13}\exp(-38000/T) \\
k_{-1} &= 1.6e^{13} \\
k_2 &= 6.4e^9T\exp(-3150/T) \\
k_{-2} &= 1.5e^9T\exp(-19500/T) \\
k_3 &= 4.1e^{13} \\
k_{-3} &= 2.0e^{14}\exp(-23650/T)
\end{align*}
\]

The equilibrium, steady-state assumptions for radicals,

1. The formation and consumption is too fast and \( N \) is considered as steady state species

\[
\frac{d\tilde{N}}{dt} = k_1(\tilde{T})[\tilde{N}_2][\tilde{O}] - k_2(\tilde{T})[\tilde{N}][\tilde{O}_2] - k_3(\tilde{T})[\tilde{OH}][\tilde{N}]
\]

\[
-k_{-1}(\tilde{T})[\tilde{NO}][\tilde{N}] + k_{-2}(\tilde{T})[\tilde{NO}][\tilde{O}] + k_{-3}(\tilde{T})[\tilde{NO}][\tilde{H}] \approx 0.
\]

2. The concentrations of \( O, OH \) are assumed to be at equilibrium hence can be correlated

\[
[\tilde{O}]_e = \frac{3.97e^2}{\tilde{T}^{1/2}}[\tilde{O}_2]^{1/2}\exp(-31090/\tilde{T}),
\]
\[ [\tilde{OH}]_e = \frac{2.129e^2}{T^{0.57}} [\tilde{O}]_e^{1/2} [\tilde{H}_2\tilde{O}]^{1/2} \exp(-4595/T). \]

So the expression for net rate is reduced to,

\[ \tilde{NO} = \frac{d\tilde{NO}}{dt} \simeq 2k_1(\tilde{T})[\tilde{O}_e][\tilde{N}_2] \left( 1 - \frac{[\tilde{NO}]^2}{K[O_2][N_2]} \right), \]

where,

\[ K = \frac{k_1}{k_{-1}} \frac{k_2}{k_{-2}}. \]
References


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Publications following during his Master project

Publications following from his PhD project


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- European Combustion Meeting, Cardiff (UK), 2011
- International Conference on Numerical Combustion, Corfu (Greece), 2011
- International Symposium on Combustion, Warsaw (Poland), 2012
- International Conference on Liquid Atomization and Spray Systems, Heidelberg (Germany), 2012
- International Conference on Numerical Combustion, San Antonio (USA), 2013
- SAE world congress, Detroit (USA), 2013