Numerical analysis on the characteristics of NOx and PM emissions using multiple injection strategies in diesel engines

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Numerical analysis on the characteristics of NOx and PM emissions using multiple injection strategies in diesel engines

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Abstract

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As the environmental concerns arise, both reduction of the emissions and increase of the efficiency have become important to achieve in the automotive industry. In addition, NOx and PM emissions from Diesel engines are more important than ever. Since NOx and PM emissions are in a trade-off relationship in conventional diesel engines, many researches have been suggested to reduce both emissions simultaneously. A multiple injection strategy is one of the alternatives and it has been widely used in diesel engines to reduce engine noise, NOx and soot formation. Nowadays, developments of the fuel injection technology such as the common-rail and piezo-actuator system can provide more precise control of the injection quantity and time under higher injection pressures. As various injection strategies become accessible, it is important to understand the interaction of each fuel stream and following combustion process under the multiple injection strategy. To investigate these complex processes quantitatively, numerical analysis using CFD is a good alternative to overcome the limitation of experiments.
The objective of this study is to develop 3-D CFD combustion models capable of analyzing the combustion and emissions phenomena under multiple injection strategies for diesel engines. The model is based on the 2-D flamelet approach and further developed from previous works to model multi-fuel streams with higher computational efficiency. The new simplification method is compared with previous assumptions showing a better accuracy in the prediction of in-cylinder pressure, heat release rate and emissions level. Furthermore, collapse of the instantaneous solution of 2-D RIF model is introduced and the quantitative criteria is suggested to apply the collapse method multiple times. Meanwhile, semi-detailed soot model is coupled with combustion model which includes the detailed chemistry of PAH species up to pyrene (A₄).

The combustion and emissions model are validated with experimental results obtained under various engine operating conditions to verify the accuracy of the models. Both NOx and PM emissions are measured in the experiments, and the actual injection profile is also measured to thoroughly verify the combustion model by using the rig experiments. The simulation results shows that the model does an accurate job of predicting the combustion and emissions characteristics as well as several parametric variations. Furthermore, the simplification method used in the model is tested under the engine conditions and the quantitative criterion of using the collapse method multiple times is provided to determine whether the model is valid to be applied in engine conditions. Most of all, quantitative analysis is possible using the combustion model, which provides an insight of the physical mechanism of emissions reduction under multiple injection strategies.

Based on the validation results, a couple of advanced injection strategies to reduce the NOx and PM emissions are numerically investigated that are difficult to conduct with experiments. The injection rate shaping strategy can change the
instantaneous injection rate under the same injection pressure by controlling the needle opening of the injector. As the needle opening becomes faster, the premixed combustion phase increases whereas the mixing controlled combustion phase decreases because more fuel is delivered into the cylinder at the beginning of the injection which promotes the air-fuel mixing with more broad region. Thus the injection rate shaping strategy still has a trade-off relationship between NO and soot emissions that the fast opening rate can reduce the NO emissions while the soot emissions is increased. Nevertheless, it is capable of changing the instantaneous injection rate, and it is much effective when applied with other operating strategies. Additional pilot injection prior to main injection can reduce the pressure rise rate as well as the NO emission when applied with the slow needle opening because the part of fuel from the main injection is injected during the pilot injection stage which decreases the combustion temperature. Furthermore, the boot injection strategy can reduce the pressure rise rate by increasing the injection duration at an early stage of the injection.

The developed model in this study can be used to propose optimal injection strategies for various engine operating conditions, and reduce the emissions level of commercial diesel engine without additional hardware changes by presenting the direction of development on injection technology.

**Keywords:** CI engine, CFD (Computational Fluid Dynamics), NOx emissions, Soot emissions, Modified 2-D Flamelet model, Multiple injection, Advanced injection strategies

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Nomenclature

A  Pre-exponent coefficient in reaction mechanism
$A_d$  Droplet cross-sectional area
$A_s$  Droplet surface area
AC  Alternating current
ASOI  After start of injection (in figure 2.4)
aTDC  After top dead center
b  Temperature exponent in the reaction coefficient (in table 2.3)
BDC  Bottom dead center
BMEP  Break mean effective pressure
bTDC  Before top dead center
$c_p$  Specific heat coefficient
$C_a$  Agglomeration constant
$C_{am}$  Virtual mass coefficient
$C_{b1}$  Bag breakup constant
$C_{b2}$  Bag breakup constant (time)
$C_{bag,i}$  Model constant (empirical) for bag breakup
$C_d$  Drag coefficient
$C_{s1}$  Stripping breakup constant
$C_{s2}$  Stripping breakup constant (time)
$C_{stripping,i}$  Model constant (empirical) for stripping breakup
CA  Crank angle
CFD  Computational Fluid Dynamics
CI  Compression Ignition
CMC  Conditional moment closure
CPU time  Computational time
CTC  Characteristic time combustion
\(d_p\)  Soot particle diameter
\(d_{\text{nucleus}}\)  Soot inception particle nucleus
\(d_{\text{PAH}}\)  Diameter of PAH species (in table 2.4)
D  Diffusion coefficient
\(D_d\)  Instantaneous droplet diameter
\(D_{d,\text{stable}}\)  Stable droplet diameter within specific time
DNS  Direct Numerical Simulation
DPF  Diesel particulate filter
\(E_a\)  Activation energy
ECFM-3Z  3-Zone Extended Coherent Flame Model
ECU  Engine control unit
EGR  Exhaust gas recirculation
EPFM  Eulerian Particle Flamelet Model
EVC  Exhaust valve close
EVO  Exhaust valve open
\(F_{am}\)  Virtual mass force
\(F_b\)  Body force
\(F_{dr}\)  Drag force
\(F_{h,i}\)  Diffusional energy flux in direction \(x_i\)
\(F_p\)  Pressure force
\(g\)  Gravitational acceleration vector
\(h\)  Chemico-thermal enthalpy
\(h\)  Heat transfer coefficient (in equation 2.4.4)
\( h_{fg} \)  Latent heat of vaporization
HACA  Hydrogen-abstraction-acetylene-addition
HCCI  Homogeneous Charge Compression Ignition
HRR  Heat Release Rate
injP  Injection pressure
I  Interaction factor of 2-D RIF model
I.C  Initial condition
IMEP  Indicated mean effective pressure
IVC  Intake valve close
IVO  Intake valve open
k  Kinetic energy
\( K_{bc} \)  Boltzmann constant [J/K]
LES  Large eddy simulation
\( \dot{m} \)  Mass source term
\( m_d \)  Mass of droplet
MI  Main injection
N  Soot number density [particle number/m³]
NEDC  New European Driving Cycle
NO  Nitric oxide
NOx  Nitrogen oxide
\( p \)  Piezometric pressure
\( p_t \)  Gas pressure
\( p_{v,s} \)  Partial pressure of droplet surface
\( p_{v,\infty} \)  Partial pressure of droplet surroundings
PAH  Polycyclic aromatic hydrocarbon
PCCI  Premixed Charge Compression Ignition
PDF  Probability density function
PI  Pilot injection
PISO  Pressure Implicit with Splitting of Operators
PL  Penetration length
PM  Particulate matter
PN  Particulate number
Po  Post injection
\( q_d \)  Heat flux on the droplet surface
\( \dot{q} \)  Volumetric flow rate of fuel
\( \dot{q}_R \)  Radiative heat flux
\( r \)  Distance vector to the axis of rotation
RANS  Reynolds-Averaged Navier-Stokes
RCCI  Reactivity Controlled Compression Ignition
RDE  Real Driving Emission
Re  Reynolds number
RIF  Representative interactive flamelet
RNG  Renormalized group
\( Sc_t \)  Turbulent Schmidt number
SMD  Sauter mean diameter
SOI  Start of injection
SOC  Start of combustion
t  Time
T  Temperature
\( T_d \)  Droplet temperature
TDC  Top dead center
THC  Total hydrocarbon emissions
u  Fluid velocity
\( \bar{u}_i\bar{u}_j \)  Reynolds stress tensor due to turbulent fluctuation
\(V_d\) Droplet volume
\(\dot{w}_i\) Mass production rate of \(i^{th}\) species
\(\text{We}\) Weber number
\(\text{WLTP}\) Worldwide harmonized Light Vehicles Test Procedure
\(\bar{X}\) Ensemble average of variable \(X\)
\(X_{OH}\) Soot oxidation coefficient by OH radical
\(y\) Mixture fraction ratio
\(Y_i\) Mass fraction of \(i^{th}\) species
\(Z\) Mixture fraction
\(Z_i\) Mixture fraction of \(i^{th}\) fuel stream
\(\bar{Z}^{\prime\prime}\) Variance of mixture fraction

**Greek symbols**

\(\Phi\) Equivalence ratio (-)
\(\varepsilon\) Eddy dissipation rate
\(\chi\) Scalar dissipation rate
\(\chi_i\) Scalar dissipation rate of \(i^{th}\) fuel stream
\(\chi_{st}\) Scalar dissipation rate at stoichiometric mixture fraction
\(\chi_{12}\) Cross scalar dissipation rate of each fuel stream
\(\bar{\chi}\) Mean scalar dissipation rate
\(\hat{\chi}_{st}\) Scalar dissipation rate conditioned at stoichiometric surface
\(\tau_{ij}\) Stress tensor
\(\mu\) Molecular dynamic viscosity
\(\mu_t\) Turbulent viscosity
\(\lambda\) Thermal conductivity
\(\lambda\) Excessive air ratio
$\rho$ Density

$\mu_{ij}$ Reduced mass

$\omega$ Angular velocity vector

$\tau$ Characteristic time scale

$\sigma_d$ Droplet surface tension

**Subscripts**

$dt$ Dwell time in figure 4.5-4.6

$i$ Coordinate index in equations (2.1.1) and (2.1.2)

$i$ Species index in equation (2.1.6)

$i$ Fuel stream index in equations (2.2.14) and (2.2.15)

$\text{inj}$ Injection duration in figure 4.5-4.6

$\text{st}$ Steady-state in figure 4.5-4.6

$\text{st}$ Stochiometric

$max$ Maximum
Chapter 1. Introduction

1.1 Background and Motivation

As the fuel economy and emissions regulations are becoming more stringent, diesel engines face a big challenge of reducing the engine-out emissions while achieving high efficiency. Since September 2017, EURO-6c regulation started to be applied to the light-duty diesel engines, and the most noticeable difference from the previous regulation is that the RDE (Real Driving Emissions) regulation is applied where the production of NOx and PM emissions under the real road condition are restricted as shown in figure 1.1. As a result, the regulation has become more stringent because the regulation limit is lower than the actual emissions over a wide engine condition including the transient operating range.

Meanwhile, global warming also strengthened regulations on carbon dioxide (CO₂), and it is closely related to the fuel economy of an engine because the engine produces the mechanical power by using the chemical energy of fossil fuel which contains carbon atoms. Figure 1.2 shows the previous performance and future targets on CO₂ emissions of light-duty vehicle and, as shown in the figure, it has become more urgent to improve the fuel economy to meet the upcoming CO₂ target.
<table>
<thead>
<tr>
<th>Regulation</th>
<th>EURO-6b</th>
<th>EURO-6c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target Date</td>
<td>2014.09</td>
<td>2017.09</td>
</tr>
<tr>
<td>Driving Cycle</td>
<td>NEDC (New European Driving Cycle)</td>
<td>WLTP (Worldwide Harmonized Light Vehicles Test Procedure)</td>
</tr>
<tr>
<td>RDE(^1)</td>
<td>Not applied</td>
<td>Conformity factor(^3)</td>
</tr>
<tr>
<td>PN(^2)</td>
<td>6.0 (\times) 10(^{12})</td>
<td>6.0 (\times) 10(^{12})</td>
</tr>
<tr>
<td>2.1</td>
<td>1.5 (from 2021.01)</td>
<td></td>
</tr>
</tbody>
</table>

1) RDE: Real Driving Emissions  
2) PN: Particulate Number  
3) Conformity factor: divergence between the regulatory limit tested in laboratory and value of RDE procedures

Figure 1.1. EURO emissions regulation in light-duty engine vehicle.

Figure 1.2. Worldwide CO\(_2\) emissions regulations.
Diesel engines are still one of the most attractive alternatives to achieve both low emissions and high fuel efficiency of the light-duty vehicle because they have the advantage of low fuel consumption. Due to a lot of worldwide issues, diesel engines have been facing numerous implications. Nonetheless, the problems are also an opportunity of engine development. Lots of previous studies have suggested to reduce emissions and increase efficiency, and they can be divided into the development of advanced combustion concept, after-treatment system [1-4] and reduction of heat and friction loss [5-8]. This study is focused on the aspect of deriving the advanced combustion concept.

In order to better understand the advanced combustion concept, it is necessary to understand the combustion and emissions characteristics of diesel engines. The main energy source of diesel engine is an auto-ignition of fuel which is directly injected into the combustion chamber [9], thus the injection pressure should remain high enough to enhance the breakup and atomization of liquid fuel and the ambient conditions in the combustion chamber must be satisfied for the auto-ignition to occur. For these reasons, diesel engines require a system with high injection pressure and high compression ratio with turbocharger.

Nevertheless, it is impossible for the fuel to be distributed completely uniform in the cylinder, which is the main cause of PM to occur. In addition, NOx is generated because the high pressure and temperature increases the combustion temperature, which is the main reason for the trade-off relationship between NOx and PM emissions to be unavoidable [9]. Therefore, it is concluded that there are two main ways to reduce both NOx and PM emissions in diesel engines; one is to form a homogeneous mixture as much as possible; the other is to lower the combustion temperature.
A variety of advanced combustion concepts have been proposed to overcome the above limitations. Figure 1.3 shows the Φ-T chart that describes the features of each combustion concept. Homogeneous Charge Compression Ignition (HCCI) combustion evenly advances the injection timing near the valve timing to enhance the homogeneity of air-fuel mixture, which reduces the PM emissions [10, 11]. In addition, the overall lean mixtures which is formed earlier than the conventional type can lower the combustion temperature, which reduces the NOx emissions. However, there are limitations to control the combustion phase because the auto-ignition occurs simultaneously in the cylinder [12]. Mixture stratification could show an enhancement on the control of combustion phase by several studies [13, 14], there are still limitations such as a load expansion to various operating conditions, combustibility problem at cold start condition [15-17]. Premixed Charge Compression Ignition (PCCI) combustion was introduced as another alternatives which can reduce both NOx and PM emissions, where the fuel and air have a sufficient time to mix each other because the ignition delay time increases due to high EGR rate and early injection timing [18]. PCCI combustion is an intermediate concept between HCCI and conventional diesel combustion, and it is a practical method because it can be achieved by single fuel and the combustion phase can be controllable if enough mixing time is available [19-22]. But it has limitations on the expansion of operating range because the EGR supply is restricted at the higher load condition and the early injection timing may cause the combustion to be instable, which results CO and unburned hydrocarbon. Dual-fuel combustion concept uses different type of fuels simultaneously in the cylinder, and promotes the in-cylinder stratification by fuel reactivity [23].

Reactivity Controlled Compression Ignition (RCCI) combustion is an alternative of HCCI combustion by using a couple of fuels [24, 25] which have a different reactivity from each other. Low reactivity fuel is supplied by the port-fuel injection or
early intake process to maintain the homogeneous characteristics of the HCCI combustion, while high reactivity fuel is directly injected to the combustion chamber during the compression stroke which works as an ignition source of low reactivity fuel. Both NOx and PM emissions are significantly reduced and the gross indicated efficiency increases in heavy-duty diesel engine, still it needs to be validated under various operating conditions for the application of automobile [26, 27]. The aforementioned combustion concepts are commonly included in the category of low temperature combustion where the temperature of combustion region is lower than that of the conventional diesel engine, and many of the other combustion concepts that belong to this have been consistently proposed. But they have a limitation on the load expansion, which cannot be directly applicable to the commercial diesel engine.

![Figure 1.3. Advanced combustion concept in Phi-T chart (original figure from Akiyama et al. [28]).](image)

On the other hand, the multiple injection strategies have been widely used to the commercial diesel engines, providing significant improvements in the fuel economy
and the reduction of emissions as well as noise and vibration [29-38]. A common-rail direction injection system enables the fuel spray to be injected with higher pressure, faster response and accurate control, which is impossible in the past mechanical injection system [39]. Thus the injection pressure and achievable number of injection have drastically increased up to 2,700 bar and 10 pulse systems [40, 41].

Figure 1.4. (a) Schematic diagram of the multiple injection system. (b) Development of injection pressure over the past century (original data obtained from [42]).
As the preceding combustion concept such as HCCI, PCCI and RCCI is realized through changes of the injection timing, the injection strategies substantially affect the combustion characteristics [43, 44]. This means that the multi-stage injection system have more potentials to achieve both emissions reduction and high engine efficiency because each injection event can be controlled independently according to its purpose. In fact, it has turned out that the multiple injection has many advantages over fuel consumption and emissions. A small amount of fuel prior to main injection, which is called pilot injection, can heat the combustion chamber and help the main injection to auto-ignite more easily [34, 35, 38]. Thus the pilot injection can reduce the NOx emissions as well as the combustion noise because it mitigates the drastic pressure rise of the main combustion. In addition, the fuel injection after the main injection, which is called a post injection, is known to significantly affect the reduction in soot emissions [45]. According to the previous research, not only it promotes the oxidation of soot emissions, but also is useful for the maintenance of after-treatment system [46]. Most of the commercial diesel engine use the multiple injection strategies including combination of the pilot, main and post injection, and the pilot and post injection are applied twice depending on the operating conditions. As a result, the injection technology will be developed in a way that can be controlled more accurately, even when a small amount of fuel is injected more frequently. Thus, it is important to develop an optimal injection strategies in line with the development of the multiple injection system.

Meanwhile, Computational Fluid Dynamics (CFD) techniques have been widely used in various engineering problems because it can visualize the parameters that are difficult to measure experimentally, and provide a quantitative analysis. Particularly in the engine, which is a high-speed mechanical system, there is a limit to empirically measure and analyze the physical phenomena occurring within a cycle. Therefore, the
CFD approach is the most suitable way to proactively investigate the optimized multiple injection strategies. In order to propose meaningful results, it is essential to ensure the reliability of the numerical models used in the analysis.

Figure 1.5. Schematic diagram of non-premixed combustion in diesel engine.

Figure 1.5 shows the overview of model composition to simulation the non-premixed flame in diesel engines. From the fuel’s point of view, which is directly injected into the cylinder; first it entrains the air stream by its injection momentum. Turbulence and spray model describe the region where the liquid fuel droplet undergoes a breakup and atomization process and the fuel vapor is mixed with air stream. The auto-ignition of fuel and air mixture occurs far from the injection points and the turbulent diffusion flame is developed and produces NOx and PM emissions. This study focuses on the modelling of combustion and emissions in case of multi-fuel stream, and the details of the model will be described in the model description (chapter 2). Thus, the multiple injection system in diesel engines will be numerically investigated using the above model composition in this paper.
1.2 Literature review

1.2.1 Turbulence modelling

Due to drastic increase of the computing power, computational modeling of the turbulence have been improving over the past few decades [47]. The simulation of the turbulent flow needs to solve the basic equations regarding mass, momentum and energy conservation. It is well known that the turbulent motion of flow consists of a number of eddies which have their own characteristic time and length, and the smallest size of the turbulent motion is called Kolmogorov length scale which is proportional to Re\(^{-3/4}\) [48]. Since Reynolds number of the turbulent flow in reciprocated engine is sufficiently high, very small grid size of the spatial domain is needed to resolve all the turbulent eddies. There are mainly three approaches according to the range of flow length scale to be solved by the model, which are Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) simulation. DNS directly solves all length scales of the turbulent eddy, and the modeling of the turbulence is not required [49]. But it has a limitation on huge CPU time, and the LES approach was suggested to satisfy the CPU time for the realistic range, which directly solves the length scale only below a certain length scale [50]. Though it has begun to be actively studied for engine research from last few years due to the increase in computational efficiency, there is still a limit to apply for the commercial engine. RANS simulation is a mathematical decomposition of Navier-Stokes equation, and the turbulent properties are fully modelled by the numerical model [51]. Therefore, it is concluded that the RANS approach is a realistic and inexpensive alternative for the engine development process.
Because the RANS equations are based on the statistical description because the turbulence is a random nature [52], the flow motion is described by the mean quantities and the turbulence model focuses on the modeling of the Reynolds stress term as a function of mean flow. The modeling of the turbulent stress has been attempted [53, 54], and the most common model is based on the transport equation regarding the turbulent kinetic energy (k) and eddy dissipation rate (ε), which is called k-ε turbulence model [55]. Then the original k-ε model was developed using renormalized group (RNG) method which has been widely used in an engine application [56].

1.2.2 Non-premixed turbulent combustion modelling

Unlike pure turbulent flow field, combustion system needs an additional equation which describes the transport of reactive scalars participating in the chemical reaction and their chemical source term. Though the RANS approach successfully solved the closure problem of Navier-Stokes equation by Reynolds decomposition and the appropriate turbulence modeling, there is a new closure problem regarding the chemical source term in the simulation of combustion phenomena because the chemical reaction is a strong non-linear function of the reactive species. Thus it is important to treat the chemical source term using appropriate assumptions, and it is one of the main objectives of the turbulent combustion modelling in a numerical point of view.

A first step to solve the closure problem of chemical source term is to describe the effect of turbulence on the chemical reaction. In the early stage, the chemical reaction was described directly by the turbulence parameter. Eddy-break-up model suggested the correlation of chemical reaction rate as function of turbulent kinetic
energy (k) and eddy dissipation rate (ε) in premixed combustion case [57], and the Shell ignition model [58] described the auto-ignition of fuel without any interaction of chemical reaction and turbulent flow. Magnussen [59] suggested a new combustion model by modelling the chemical reaction rate as a function of turbulent kinetic energy, dissipation rate and mean quantity of reactive species. However, in certain situations, the earlier models overestimate the reaction rate because the chemical reaction is infinitely fast and always reach a chemical equilibrium [60]. Therefore, the combustion behavior after the auto-ignition could not be predicted by the model when it comes to the application of diesel engines.

Characteristic Time Combustion (CTC) model is a developed version of the eddy-breakup model [61], which describes the turbulence with finite-rate chemistry as an Arrhenius form by introducing the characteristic time related to turbulence mixing. Even though it is considered an acceptable result in wide applications of diesel engines, Singh and Reitz revealed that it could not predict the intermediate species under low temperature combustion regime [62]. Conditional Moment Closure (CMC) model is another advanced combustion model for non-premixed flame where the chemical source term is conditionally-averaged and modelled by the conditional moment [63]. However, the computational time and memory requirements of CMC model are rather high for engine applications despite of its advantage in having a better prediction of non-premixed flame [64].

A laminar flamelet approach [65] is the most popular concept of turbulent-chemistry interaction where the combustion occurs in a small layer which is thin compared to the turbulent eddy size, and only one conserved scalar which is denoted as mixture fraction Z in previous works can describe the non-premixed diffusion flame by coordinate transformation based on the thin reaction layer assumption. The turbulent effect is reflected in the flamelet equation by the scalar dissipation rate (χ)
which means the characteristic diffusion time, but it cannot predict the transient behavior of the turbulence effect because it did not consider the temporal change of scalar dissipation rate and only considered a function of mixture fraction instead. It has been extended to Representative Interactive Flamelet (RIF) concept to simulate the unsteady diffusion flame where the scalar dissipation rate is calculated by reflecting the instantaneous turbulent flow field at each time [66], and it showed a successful agreement with experimental results of diesel combustion [67]. RIF model was additionally extended to the multiple formulation form called Eulerian Particle Flamelet Model (EPFM), where a number of flamelet solution having different time histories can describe the combustion phenomena by dividing the entire domain according to the eulerian marker. EPFM concept showed better prediction of non-premixed flame in diesel engine application [68]. The RIF model is a base concept of this study, and it will be discussed in the model description section with details of model formulation.

The above combustion models of non-premixed turbulent flame have been further developed for engine simulation by applying various approaches such as transported probability density function (PDF) [69], progress-variable approach [70], etc., and the each combustion model has its own advantages and disadvantages. Thus the one who wants to simulate the non-premixed combustion should choose an appropriate model for the modelling purpose with considering the validity of each combustion model.

1.2.3 Numerical investigation of multiple injection strategies

As mentioned in the previous section, one must identify the characteristics of each combustion model in order to select a model suitable for the purpose of the
multiple injection strategies. Unlike premixed combustion, the combustion takes place in after mixing of fuel and oxidizer at the molecular level in turbulent non-premixed combustion, and it is important to figure out whether the mixing can affect the chemical reactions or not. Thus the combustion model can be classified into two parts depending on the calculation of interaction between turbulent flow field and chemical reaction rates, as listed below.

(1) Chemical reaction is calculated with directly considering the effect of turbulence field on the chemical reaction at each spatial domain - CTC model, direct integration method [71], ECFM-3Z model [72], etc.

(2) Chemical reaction is calculated apart from the flow field by introducing the assumptions where mathematical derivations and can be included - RIF model, CMC model, transported PDF model and EPFM model, etc.

For the case of direct calculation on chemical kinetics, the calculation time is closely dependent on both the number of grid point and the size of chemistry because each reaction rate is calculated at each cell by cell. On the other hand, combustion model which calculate the chemical reaction separating from the flow field can reduce the CPU time and thus adapt more complex chemistry for the better prediction of combustion process. It is different when it comes to modelling the non-premixed flame by multiple fuel stream because more appropriate assumptions and modelling are needed for the second type of combustion model.

For this reason, a lot of numerical researches of multiple injection strategies have been investigated by using the direct calculation method at an early stage. The effects of multiple injection on NOx and soot emissions were investigated by using CTC model coupled with KIVA-II software [35, 73]. In the 1990s, researches of the
multiple injection focused on the experimental approach, and the numerical investigation became active in the 2000s due to the increase of computing power and the development of numerical techniques. A number of studies to calculate both chemistry and flow field together have still been suggested [11, 74, 75] to simulate the non-premixed combustion of diesel engine, but there is a fundamental limitation on the increase in the size of chemistry due to the restricted CPU time.

There also has been a development of the model to describe the combustion process under multi-fuel stream while chemistry is separately solved from the turbulent flow field. CMC model has been extended to mimic the combustion system which consists of two fuel streams and a single oxidizer stream [76-78], and showed a good agreement with experimental results using the two pulse injection system.

RIF model, which was used in this study, has been extended to its two-dimensional form by introducing the three-scale asymptotic analysis [79], which is called 2-D RIF model. Unlike the conventional RIF model, the governing equations of 2-D RIF model are constructed by the two mixture fractions and the interaction of each fuel spray can be described by the 2-D RIF model. Numerical researches using the 2-D RIF model nicely captured the combustion process of two pulse injection system, however, the computational time was drastically increased because the number of grid point in the flamelet solution domain increases dozen of times.

To overcome the limitations of CPU time, 2-D RIF model was simplified by neglecting the calculation process of overly lean and rich region [80]. The idea is based on the fact that the auto-ignition of fuel mainly occurred near stoichiometric region and the convection and diffusion term in the governing equations are dominant in extremely rich or lean region. Even though the model has successfully reduced the CPU time without any large discrepancies with the original 2-D RIF model, the model
was validated by comparing only the ignition delay time experimented under constant volume vessel. It was applied to the engine condition of PCCI combustion in diesel engine, the combustion process showed a slightly different behavior with experimental results [81].

Another limitation of 2-D RIF model is that it can only describe two fuel streams which is not able to be applied to the real engine application, because the most of commercial diesel engine uses the injection strategies including more than three injection events. Thus the extended 2-D RIF model was suggested by introducing the method of solution collapse where the present two dimensional solution is collapsed to one-dimension before the third injection, because it is sufficiently reasonable when the instantaneous solution of flamelet equation have already reached a steady-state [82]. Simulation of third fuel stream became possible by this model, and the model was applied to the engine conditions having three pulse injection strategies. The solution should be able to be repeated several times to apply more large number of injection for the further application, but the study on detailed verification of collapse method has not been conducted.

1.2.4 Modelling of soot formation in diesel engines

Unlike the NOx emissions, soot particle is made of a solid carbon group and known to be a necklace-like agglomerate [83], and the modelling of soot formation in diesel engine is still a challenging work because the formation and oxidation processes are not completely understood and numerous factors contribute to the soot formation such as equivalent ratio, temperature and fuel properties, even though there are lots of attempts to describe the production of soot particle.
The most widely known model of the soot formation was suggested by Hiroyasu et al. [84] which describes the soot formation and oxidation by simple one-equation, and the initial formation of soot emissions was directly represented by the fuel concentration while the oxidation was directly related to the oxygen concentration.

Since the one-equation model did not consider the detailed process of soot formation which overestimated the soot emissions due to lack of description in oxidation process via OH radicals, the following research has subdivided the soot formation process into several steps such as nucleation, surface growth, coagulation and agglomeration [85], and the detailed modelling approaches of each step were suggested. These procedures can be divided into two pathway: gas-phase reactions from the fuel pyrolysis to the formation of soot precursors and the particle dynamics which determine the formation of soot particle, its size and number. As a first step of soot formation, the formation of soot precursor from the fuel pyrolysis was generally assumed by acetylene (C₂H₂) and polycyclic aromatic hydrocarbon (PAH) [84, 86-89] because it has been found to be abundant in the soot formation region. In early stage, the soot nucleation was simply described by only acetylene [86, 90-93], however, it could not fully explain the process from the fuel pyrolysis to the formation of soot precursor. A first attempt to consider the PAH as initial reaction of the soot formation was performed by Frenklach [94], and a more detailed approach could be possible due to the reaction pathways of surface growth via PAH species which is well-known as hydrogen-abstraction-acetylene-addition (HACA) mechanism. Afterward, a lot of semi-detailed approaches were suggested by combining the detailed chemistry of PAH and soot particle dynamics [95-97], and they showed more improved agreement with experimental results than simple empirical model.

On the other hand, the soot oxidation process is relatively simple reaction pathway and it can be occurred throughout the soot formation process. There have
been reported that a lot of species can affect the soot oxidation in fuel-lean condition [98], it is mainly occurred by oxygen and OH radicals at high temperature environment like in diesel engines. For the oxidation process via oxygen molecules, the well-known semi-empirical model was suggested by Nagle and Strickland-Constable [99], and the oxidation of soot emissions by OH radicals become more important in the fuel-rich condition because the oxidation rate of soot emissions does not much affected by the partial pressure of oxygen molecule [100, 101].

In this study, semi-empirical model suggested by vishwanathan et al [96] was used because it is a practical model which include both detailed reaction pathways of PAHs up to A₄ (pyrene) and time-efficient modelling from the PAH species to final soot emissions.
1.3 Objectives

As seen earlier, the multiple injection strategy is an essential option for the advanced combustion to meet the emissions regulation, and still it has a potential to further reduce both emissions with higher efficiency. In order to reach an optimal injection strategy, it is important to investigate the physical phenomena of turbulent non-premixed combustion under the multi-fuel stream. Therefore, this paper focuses on the development of combustion model which describes the combustion process of various multiple injection strategies with reasonable calculation time so that it can be applicable to the engine development process.

The key objectives of this study can be summarized as follows:

1. Development of a robust and time-efficient model to predict the combustion and emissions characteristics under the multiple injection strategies of diesel engines.

2. Numerical implementation of semi-empirical soot model to the combustion model in order to predict the soot emissions under multi-fuel system

3. Validation of the combustion and emissions model by comparing with experimental results under engine operating conditions using various multiple injection strategies

4. Numerical investigation of advanced injection strategies to achieve both emissions reduction and low fuel consumption.
1.4 Structure of the thesis

This study consists of six chapters. To start off, a brief literature review on the turbulent combustion modelling and multiple injection strategies is given, and the numerical configuration of the model is provided in chapter 2. It includes the algebraic expression of the basic principle on turbulent flow, non-premixed combustion, fuel chemistry with NOx and soot emissions and liquid spray behavior. The flamelet approach is used to predict the non-premixed turbulent combustion in this study, and the mathematical derivation to apply to the multi-fuel stream is introduced as well as the history of the model in detail. In addition, the key features of the modelling methodology to mimic the large number of fuel injection with reasonable CPU time. The engine experiment is performed under various operating conditions, and the rig-experiment is followed to measure the actual injection rate which has similar condition with multiple injection strategies used in engine experiment and obtain the spray cone angle needed to input to the spray model. The other experimental data supported by Engine Combustion Network (ECN) is also used to validate the spray model by comparing the penetration length. Both experimental and computational setup to validate the combustion model is presented in chapter 3. In chapter 4, validation results of the combustion and emissions model is quantitatively discussed through the evaluation of consistency with engine experimental data. Based on the results, optimal injection strategies are suggested to find the improvement on the reduction in both NOx and soot emissions while maintain the thermal efficiency in chapter 5. Finally, the conclusions and discussions of the future works of this study are briefly summarized in chapter 6.
Chapter 2. Model description

2.1 Description of flow field

2.1.1 Turbulence model

This study focuses on the internal flow of the combustion chamber in a diesel engine which is turbulent, unsteady and incompressible with high Reynolds number. The governing equations of mass and momentum conservation are described as equations (2.1.1) and (2.1.2) [102].

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = \dot{m} \tag{2.1.1}
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j - \tau_{ij})}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \dot{M}_i \tag{2.1.2}
\]

Where, \( t \) : time

\( x_i \) : Cartesian coordinate (i= 1, 2, 3)

\( u_i \) : absolute fluid velocity component in direction

\( p \) : piezometric pressure

\( \tau_{ij} \) : stress tensor

\( \dot{m} \) : mass source term

\( \dot{M}_i \) : momentum source term in direction

\( \rho \) : density of fluid

The governing equations of RANS simulation can be derived by Reynolds decomposition, and the solution variables in equations (2.1.1) and (2.1.2) become ensemble averaged form [51].
\[ \frac{-\rho u_i}{\rho} \frac{\partial u_i}{\partial x_j} = \rho M_j + \frac{\partial}{\partial x_j} \left( \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_k} \delta_{ij} \right) - \rho u_i u_j \]  

(2.1.3)

Where,  
\( \mu \) : molecular dynamic viscosity  
\( \overline{u_i u_j} \) : Reynolds stress tensor due to turbulent fluctuation  
\( \overline{X} \) : ensemble average of variable X

A k-\( \varepsilon \) with the renormalization group (RNG) was used to make the equation (2.1.3) become closure. It is a kind of two-equation model which solves the turbulent kinetic energy and eddy dissipation rate, and each parameter describes the turbulent velocity scale and length scale respectively as shown in equations (2.1.4) and (2.1.5). Detailed information of the empirical coefficients used in the model is listed in table 2.1.

\[
\begin{align*}
\frac{\partial (\rho k)}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho u_i k - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right) &= \mu_t (P + P_g) - \rho \varepsilon \left( \mu_t \frac{\partial u_i}{\partial x_j} + \rho k \right) \frac{\partial u_i}{\partial x_j} \\
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho u_i \varepsilon - \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right) &= C_{\varepsilon 1} \frac{\varepsilon}{k} \left[ \mu_t \left( \frac{P - \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_j} + \rho k \right) \frac{\partial u_i}{\partial x_j} \right) \right] \\
-C_\varepsilon \rho \frac{\varepsilon^2}{k} + C_{\varepsilon 3} \frac{\varepsilon}{k} \mu_t P_g + C_{\varepsilon 4} \rho \varepsilon \frac{\partial u_i}{\partial x_j} - \frac{\rho \varepsilon^2}{k} C_{\varepsilon 3} \mu_t (1 - \mu / \mu_0) \frac{1 + \beta \eta}{1 + \beta \eta} \quad (2.1.5)
\end{align*}
\]

Table 2.1. Coefficients of the RNG k-\( \varepsilon \) turbulence model

<table>
<thead>
<tr>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\varepsilon )</th>
<th>( \sigma_h )</th>
<th>( C_{\varepsilon 1} )</th>
<th>( C_{\varepsilon 2} )</th>
<th>( C_{\varepsilon 3} )</th>
<th>( C_{\varepsilon 4} )</th>
<th>( \eta_0 )</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.085</td>
<td>0.719</td>
<td>0.719</td>
<td>0.9</td>
<td>1.42</td>
<td>1.68</td>
<td>0.0*</td>
<td>-0.33</td>
<td>4.38</td>
<td>0.012</td>
</tr>
</tbody>
</table>

* \( C_{\varepsilon 3} = 1.42 \) for \( P_g > 0 \)
2.1.2 Transport equation of enthalpy and scalar

In order to calculate the combustion phenomena, it is necessary to solve the transport of the enthalpy of mixture and reactive scalars participating in the chemical reaction, and the enthalpy of the combustion system is a sum of thermal enthalpy and chemical species.

\[ h \equiv c_p T - c_p^0 T_0 + \sum Y_i h_i \]  \hspace{1cm} (2.1.6)

Where,
- \( h \): chemico-thermal enthalpy
- \( \overline{c_p} T \): Reynolds stress tensor due to turbulent fluctuation
- \( c_p^0 T_0 \): heat capacity at reference temperature \( T_0 \)
- \( Y_i \): mass fraction of \( i \)th species
- \( h_i \): heat of formation of \( i \)th species

Based on the definition of enthalpy in equation (2.1.6), the total energy is balanced in the cylinder with considering the chemical reactions and fluid heat transfer by the equation (2.1.7).

\[ \frac{\partial (\rho h)}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho u_j h + F_{h,i} \right) = \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \tau_{ij} \frac{\partial u_j}{\partial x_i} + \dot{s}_h \]  \hspace{1cm} (2.1.7)

Where,
- \( F_{h,i} \): diffusional energy flux in direction \( x_i \)
- \( \dot{s}_h \): enthalpy source term

In the same way, additional conservation equation of arbitrary scalar is needed to describe the chemical reaction, and the mixture fraction was chosen as a conserved scalar. The conservation equation of mixture fraction was suggested by Peters [65], as shown in equation (2.1.8).
\[
\frac{\partial (\rho Z)}{\partial t} + \frac{\partial}{\partial x_i} \left[ \rho u_i Z - \left( \rho D_i + \frac{\mu_i}{S_c_i} \frac{\partial Z}{\partial x_i} \right) \right] = \dot{s}_Z \tag{2.1.8}
\]

Where, \( Z \) : mixture fraction
\( S_c_i \) : turbulent Schmidt number
\( \mu_i \) : turbulent viscosity
\( \dot{s}_Z \) : source term of mixture fraction

### 2.2 Turbulent combustion model

#### 2.2.1 Laminar flamelet model

The laminar flamelet concept [65] has been widely used to predict the non-premixed combustion as mentioned in the literature review. The governing equations regarding the chemical species and enthalpy are described in the physical domain by equations (2.2.1) and (2.2.2).

\[
\rho \frac{\partial (\rho Y_i)}{\partial t} + \rho u_i \frac{\partial Y_i}{\partial x_a} = \frac{\partial}{\partial x_a} \left( \rho D_i \frac{\partial Y_i}{\partial x_a} \right) + \dot{w}_i \tag{2.2.1}
\]

\[
\rho \frac{\partial h}{\partial t} - \frac{\partial}{\partial x_a} \left( \lambda \frac{\partial h}{\partial x_a} \right) = -\frac{\partial}{\partial x_a} \sum_i h_i \left( \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial x_a} - \rho D_i \frac{\partial Y_i}{\partial x_a} \right) + \frac{\partial p}{\partial t} + \dot{q}_r \tag{2.2.2}
\]

Where, \( Y_i \) : mass fraction of \( i^{th} \) species
\( D \) : diffusion coefficient
\( \lambda \) : thermal conductivity
\( \dot{q}_r \) : radiative heat flux
\( \dot{w}_i \) : mass production rate of \( i^{th} \) species
The concept of laminar flamelet model can be described by introducing the two main parameters, mixture fraction ($Z$) and scalar dissipation rate ($\chi$). In a two-feed combustion system (i.e. fuel stream and oxidizer), the mixture fraction is defined by the equation (2.2.3), and it is a conserved scalar because the chemical reaction ensures the mass conservation of chemical species before and after the reactions. For convenience, definition of mixture fraction will be followed by equation (2.2.3) in this study because we only focus on the combustion system of diesel engines which consists of pure fuel stream and oxidizer stream.

$$Z = \frac{m_{\text{fuel}}}{m_{\text{oxidizer}} + m_{\text{fuel}}} \quad (2.2.3)$$

In the laminar flamelet model, it was assumed that the chemical reaction occurs at the vicinity of stoichiometric flame surface in non-premixed combustion, the new coordinate was attached at the normal direction to the flame surface and the balance equations (2.2.1-2.2.2) was newly described by the mixture fraction using the coordinate transformation. The $Z$ was set to the normal direction of flame surface, and the other two axis (denote $Z_2$ and $Z_3$) were set to the tangential direction of flame surface in the new coordinate system. The assumption of the thin reaction zone makes the derivative terms regarding $Z_2$ and $Z_3$ much smaller than that of mixture fraction $Z$, and these low order term can be neglected. Then the balance equation turns into a one-dimensional form regarding the mixture fraction as shown in equations (2.2.4-2.2.5) where the Lewis number is assumed to be unity.

$$\frac{\partial Y_i}{\partial t} = \frac{1}{2Le_i} \left( \chi \frac{\partial^2 Y_i}{\partial Z^2} \right) + \frac{\dot{m}_i}{\rho} \quad (2.2.4)$$
\[
\frac{\partial T}{\partial t} - \frac{1}{2} \left( \chi \frac{\partial^2 T}{\partial Z^2} \right) - \chi \frac{\partial T}{c_p} \left[ \sum_{i=1}^{N} c_{i\alpha} \frac{\partial Y_i}{\partial Z} + \frac{\partial c_{i\alpha}}{\partial Z} \right] = \frac{1}{\rho c_p} \left\{ \frac{\partial p}{\partial t} - \dot{q}_r - \sum_{i=1}^{N} \dot{m}_i h_i \right\}
\]

(2.2.5)

\[
\chi = 2D \left( \frac{\partial Z}{\partial \alpha} \right)^2
\]

(2.2.6)

Another important parameter which was introduced in the equations (2.2.4-2.2.5) is the scalar dissipation rate \((\chi)\), and it is defined by equation (2.2.6). It is reflected by the form of the diffusion coefficient in equation (2.2.4-2.2.5), and it describes the effect of turbulence on the flamelet equations. In Peter’s research [65], it can be represented by a mixture fraction dependency in the laminar counter-flow diffusion flame with constant density, as shown in equation (2.2.7).

\[
\chi(Z) = \frac{a}{\pi} \exp \left\{ -2 \left[ \text{erfc}^{-1}(2Z) \right]^2 \right\}
\]

(2.2.7)

Above governing equations were also derived by using an asymptotic analysis [79], and another expression of scalar dissipation rate was also suggested by Pitsch [103] based on the logarithmic correlation using the maximum mixture fraction, as given in equation (2.2.8).

\[
\chi(Z) = \chi_{st} \frac{Z^2}{Z_{st}^2} \frac{\ln(Z / Z_{\text{max}})}{\ln(Z_{st} / Z_{\text{max}})}
\]

(2.2.8)

It is still to describe the scalar dissipation rate at the stoichiometric mixture fraction because it was not represented by the turbulence parameter in non-premixed environment but derived by assumptions of particular flow condition. In order to apply flamelet equations to the general turbulent non-premixed combustion, the scalar
dissipation rate in equation (2.2.8) was density-averaged as equation (2.2.9), and the first integral in right-hand side of equation was defined as the mean scalar dissipation rate conditioned on stoichiometric mixture fraction \([104]\).

\[
\tilde{\chi} = \tilde{\chi}(Z) = \int_{Z_{st}} \tilde{\chi}_{st} \tilde{P} \tilde{\chi}_{st} d\tilde{\chi}_{st} \int_{Z} f(Z) \tilde{P}(Z) dZ \tag{2.2.9}
\]

Here the function \(f(Z)\) is a form of error function or logarithmic function, and each parameter was assumed to be statistically independent in equation (2.2.9). The probability density function was presumed by the beta function which consists of the mean and variance of the mixture fraction distribution which is suggested by Girimaji [105].

\[
\tilde{P}(Z) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} Z^{\alpha-1}(1-Z)^{\beta-1}
\]

\[
\alpha = \frac{\tilde{Z}(1-\tilde{Z})}{Z^2} \cdot \beta = \frac{\tilde{Z}(1-\tilde{Z})}{Z^2} - 1 \tag{2.2.10}
\]

where \(\Gamma(\alpha) = \int_{0}^{\infty} x^{\alpha-1} e^{-x} dx\)

And the mean scalar dissipation rate \(\tilde{\chi}\) was calculated by turbulence parameter

\[
\tilde{\chi} = c_{\chi} \tilde{Z}^{-2} \tag{2.2.11}
\]

where \(c_{\chi}\) is 2.0 [106].

Combining both equation (2.2.9) and (2.2.11) gives the description of the conditional averaged scalar dissipation rate at a local point, and again it is averaged over a whole computational domain to provide a single parameter which could be applied in the flamelet equations for the turbulent non-premixed combustion, as shown in equation (2.2.12)
Finally, domain-averaged scalar dissipation rate conditioned at the surface of the stoichiometric mixture is used to calculate the scalar dissipation rate as a function of mixture fraction which can be applied to the flamelet equation. The representative interactive flamelet (RIF) concept [66] links the solution of flamelet equation with the instantaneous flow field where the scalar dissipation rate is calculated by the information of flow field updated at each time and applied to the governing equations of laminar flamelet model, as shown in figure 1.6.

\[
\langle \chi_n \rangle = \int_{z_a} \chi_n \tilde{p}(\chi_n) d\chi_n = \frac{c_e \tilde{\gamma} \tilde{k} \tilde{Z}^2}{\int f(Z) \tilde{p}(Z) dZ} \tag{2.2.12}
\]

\[
\langle \chi_n \rangle = \int_{z_a} \chi_n \tilde{p}(Z_a) dV = \frac{c_e \tilde{\gamma} \tilde{k} \tilde{Z}^2}{\int f(Z) \tilde{p}(Z) dZ} \tag{2.2.13}
\]
Figure 2.1. Calculation structure of RIF concept.
2.2.2 Flamelet model for multi-fuel stream

Conventional RIF model has been extended to mimic the non-premixed combustion of multi-fuel stream. Since the original model was based on single mixture fraction, it is essential to derive the new governing equation based on two mixture fraction variables in case of three-feed system (i.e. two fuel streams and one oxidizer stream). Using the three-scale asymptotic analysis, the governing equations of the two-dimensional RIF model was derived with unity Lewis number [79].

\[
\frac{\partial Y_i}{\partial t} = \frac{1}{2} \left( \chi_i \frac{\partial^2 Y_i}{\partial Z_i^2} + 2 \chi_{i2} \frac{\partial^2 Y_i}{\partial Z_i Z_2} + \chi_2 \frac{\partial^2 Y_i}{\partial Z_2^2} \right) + \frac{m_i}{\rho} \tag{2.2.14}
\]

\[
\frac{\partial T}{\partial t} - \frac{1}{2} \left( \chi_i \frac{\partial^2 T}{\partial Z_i^2} + \chi_{i2} \frac{\partial^2 T}{\partial Z_i \partial Z_2} + \chi_2 \frac{\partial^2 T}{\partial Z_2^2} \right) - \frac{1}{c_p} \left[ \sum_{i=1}^{N_f} c_{c_p,i} \left( \chi_i \frac{\partial Y_i}{\partial Z_i} + \chi_{i2} \frac{\partial Y_i}{\partial Z_2} \right) + \chi_1 \frac{\partial c_p}{\partial Z_1} + \chi_{i2} \frac{\partial c_p}{\partial Z_2} \right] - \frac{1}{c_p} \left[ \sum_{i=1}^{N_f} c_{c_p,i} \left( \chi_2 \frac{\partial Y_i}{\partial Z_2} + \chi_{i2} \frac{\partial Y_i}{\partial Z_2} \right) + \chi_2 \frac{\partial c_p}{\partial Z_1} + \chi_{i2} \frac{\partial c_p}{\partial Z_2} \right] = \frac{1}{\rho c_p} \left( \frac{\partial \rho}{\partial t} - \dot{q}_c - \sum_{i=1}^{N_f} \dot{m}_i h_i \right) \tag{2.2.15}
\]

\[
\chi_1 = 2D \left( \frac{\partial Z_1}{\partial x_a} \right)^2 \quad \chi_2 = 2D \left( \frac{\partial Z_2}{\partial x_a} \right)^2 \quad \chi_{i2} = 2D \left( \frac{\partial Z_i}{\partial x_a} \frac{\partial Z_2}{\partial x_a} \right) \tag{2.2.16}
\]

Where,  
\( Z_i \) : mixture fraction of \( i \)th fuel stream  
\( \chi_i \) : scalar dissipation rate of \( i \)th fuel stream  
\( \chi_{i2} \) : cross scalar dissipation rate of each fuel stream
Equations (2.2.14-2.2.15) is a multi-dimensional form of flamelet equations by introducing the two mixture fraction $Z_1$ and $Z_2$. Additionally, the scalar dissipation rate needs to be derived under the multi-fuel environment with appropriate assumption of joint scalar dissipation rate $\chi_{12}$. For $\chi_1$ and $\chi_2$, previous research showed that the spatial gradient of each scalar which is a right-hand side of equation (2.2.16) is not affected by each other, and they are represented as similar description of equation (2.2.7).

$$\chi_1(Z_1, Z_2) = \frac{a_1}{\pi}(1-Z_2)\exp\{-2\left[\text{erfc}^{-1}(2Z_1/(1-Z_2))\right]^2\}$$ \hspace{1cm} (2.2.17)$$

$$\chi_2(Z_1, Z_2) = \frac{a_2}{\pi}(1-Z_1)\exp\{-2\left[\text{erfc}^{-1}(2Z_2/(1-Z_1))\right]^2\}$$ \hspace{1cm} (2.2.18)

The modelling of joint scalar dissipation rate $\chi_{12}$ was suggested to consider the mixing along the boundary at $Z_1 + Z_2 = 1$ by introducing the third mixture fraction $Z_3 = 1 - Z_1 - Z_2$ \cite{107, 108}. But the other DNS research showed that the consideration of the joint scalar dissipation rate could not show a large difference \cite{109}, thus it was neglected in this study.

Because the solution domain of the 2-D flamelet equations has a constraint where $Z_1 + Z_2 = 1$, it becomes a triangular shape which might cause a numerical problem. Thus the new variables were introduced and the governing equations are constructed \cite{79} by coordinate transformation with neglecting the joint scalar dissipation rate, as shown in equation (2.2.19-2.2.21).

$$Z = Z_1 + Z_2, \ y = Z_1 / (Z_1 + Z_2)$$ \hspace{1cm} (2.2.19)
\[
\frac{\partial Y}{\partial t} = \frac{X_1}{2} \left( \frac{\partial^2 Y}{\partial Z^2} + 2 \frac{y}{Z} \frac{\partial^2 Y}{\partial Z \partial y} - 2 \frac{y^2}{Z^2} \frac{\partial^2 Y}{\partial y^2} \right) + \frac{X_2}{2} \left( \frac{\partial^2 Y}{\partial Z^2} + 2 \frac{(1-y)}{Z} \frac{\partial^2 Y}{\partial Z \partial y} - 2 \frac{(1-y)^2}{Z^2} \frac{\partial^2 Y}{\partial y^2} \right) = \frac{\dot{h}_i}{\rho} \tag{2.2.20}
\]

\[
\frac{\partial T}{\partial t} = \frac{X_1}{2} \left( \frac{\partial^2 T}{\partial Z^2} + 2 \frac{y}{Z} \frac{\partial^2 T}{\partial Z \partial y} - 2 \frac{y^2}{Z^2} \frac{\partial^2 T}{\partial y^2} \right) + \frac{X_2}{2} \left( \frac{\partial^2 T}{\partial Z^2} + 2 \frac{(1-y)}{Z} \frac{\partial^2 T}{\partial Z \partial y} - 2 \frac{(1-y)^2}{Z^2} \frac{\partial^2 T}{\partial y^2} \right) + \frac{1}{c_p} \left( \frac{\partial T}{\partial y} - \frac{\partial \tilde{c}}{\partial y} \right) \sum_{i=1}^{N} c_{pi} \left( \frac{\partial Y_i}{\partial Z} - \frac{\partial \tilde{c}}{\partial T} \right) + \frac{1}{c_p} \left( \frac{\partial T}{\partial y} - \frac{1}{\rho} \dot{h}_i \right) \tag{2.2.21}
\]

The calculation procedure of each scalar dissipation rate is similar to that of one dimensional equations except the probability density function which should be revised for the multi-variable form, and the coordinate transformation of \((Z, y)\) domain is applied to the multi-variable probability density function, which is the same method with previous works \([82, 107, 110]\).

\[
\tilde{P}(Z_1, Z_2) = \frac{\Gamma(\alpha + \beta + \gamma)}{\Gamma(\alpha) \Gamma(\beta) \Gamma(\gamma)} Z_1^{\alpha-1} Z_2^{\beta-1} (1 - Z_1 - Z_2)^{\gamma-1}
\]

\[
\alpha = \tilde{Z}_1 \left[ \frac{(1-S)}{Q} - 1 \right], \quad \beta = \tilde{Z}_2 \left[ \frac{1(1-S)}{Q} - 1 \right], \quad \gamma = (1 - \tilde{Z}_1 - \tilde{Z}_2) \left[ \frac{1(1-S)}{Q} - 1 \right] \tag{2.2.22}
\]

\[
S = \tilde{Z}_1^2 + \tilde{Z}_2^2 + (1 - \tilde{Z}_1 - \tilde{Z}_2)^2, \quad Q = \tilde{Z}_1^2 + \tilde{Z}_2^2 + (\tilde{Z}_1 + \tilde{Z}_2)^2
\]

\[
\tilde{P}(Z, y) = \frac{\Gamma(\alpha + \beta + \gamma)}{\Gamma(\alpha) \Gamma(\beta) \Gamma(\gamma)} Z^{\alpha-1} y^{\beta-1} (1 - y)^{\gamma-1} \tag{2.2.23}
\]
2.2.3 Simplification of 2-D RIF model

The biggest drawback of 2-D RIF model is that the computational time increases by a factor of ten because the time needed to solve the chemical reaction increases as the number of grid of the solution domain increases. Since it takes the longest time to solve the chemical source term within the governing equation (figure 2.2), 2-D RIF model was simplified by neglecting the calculation process of chemical reaction on the region where the auto-ignition is difficult to occur, such as extremely lean or rich region [80] where the criteria for dividing the area are as follows, which is called modified 2-D RIF model.

(1) Region of $0.033 < Z < 0.08$ : governing equations of 2-D RIF model (equations (2.2.20-21)) are solved.

(2) Region of $Z < 0.033$ and $Z > 0.08$ : governing equations of 2-D RIF model are solved without source term until the temperature at $Z=0.033$ or $Z=0.08$ exceeds 2000 K.

(3) Region of $Z = 0.033, 0.08$ : governing equations (2.2.20-21) are solved except the terms regarding mixture fraction $Z$.

Even though the simplification method in [80] shows a reasonable agreement on the ignition delay time with experimental results under constant volume vessel, further improvement is required to apply for engine combustion simulation because the ignition delay time can only reflect the time when the combustion started without any effect of turbulent mixing. Therefore, it is important to verify the simplification method to apply the modified 2-D RIF model to the diesel engine simulation.
The main consideration is about how to solve the region (3) (i.e. lean and rich region) efficiently, and previous assumption has a limitation to predict the combustion phenomena under a couple of conditions because this assumption does not pertain if there is two fuel streams with small amount of fuel stream under EGR-diluted condition. Under this condition, the ignition delay of first fuel spray increases and the one-dimensional flamelet solution may not reach the steady-state at the beginning of the next injection where the substitution of the solution at $0 < y < 1$ may not be occurred because the temperature could not reach the 2000 K, which is the criteria of solution substitution. The assumption is not valid any more when the dwell time between each injection is relatively short, because there is not enough time for the first fuel stream to reach the steady-state. A new simplification method is suggested which considers the energy transfer of the solutions at $0 < y < 1$ by linear interpolation of the solutions at each fuel stream at every time step, and the solutions at $0 < y < 1$ are replaced by the solution of the first fuel stream (i.e. $y=0$) when the certain criteria is satisfied, and the criteria is changed which the solution is replaced when the temperature solution at the boundary ($Z=0.033$ and 0.08) reaches 99% of temperature at the first fuel stream, as shown in figure 2.2.

$$\sum_i h_i Y_i(Z, y)_{@0\text{cycle}} = (1 - y) \left( \sum_i h_i Y_i(Z, y = 0) \right) + y \left( \sum_i h_i Y_i(Z, y = 1) \right) \quad (2.2.24)$$
Figure 2.2. Simplification method of 2-D RIF model.
In order to verify the new simplification method of 2-D RIF model, simulation is conducted under the multiple injection in constant volume space. The ambient temperature and pressure are 900K and 40 bar, respectively, and the oxygen concentration is 13% which is a condition of low temperature combustion. Two injection strategies are tested to verify the simplification of 2-D RIF model suggested in this study, and details are listed in table 2.2.

**Table 2.2. Simulation condition for the verification of simplification**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh type</td>
<td>3-D box mesh (54mm x 54mm x 108mm)</td>
</tr>
<tr>
<td>Spray model</td>
<td>Base concept: Lagrangian approach</td>
</tr>
<tr>
<td></td>
<td>Breakup: Reitz-Diwakar model [111]</td>
</tr>
<tr>
<td>Combustion model</td>
<td>Full 2-D RIF model [79] (denote ‘Full’)</td>
</tr>
<tr>
<td></td>
<td>Modified 2-D RIF model [80] (denote ‘Modified’)</td>
</tr>
<tr>
<td></td>
<td>New 2-D RIF model (this study) (denote ‘Present’)</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>900 K</td>
</tr>
<tr>
<td>Ambient pressure</td>
<td>40 bar</td>
</tr>
<tr>
<td>Oxygen content</td>
<td>O$_2$ = 13 % (volume)</td>
</tr>
<tr>
<td>Fuel type</td>
<td>Normal heptane (nC$<em>7$H$</em>{16}$)</td>
</tr>
<tr>
<td>Injection strategies</td>
<td>Dual injection strategy</td>
</tr>
<tr>
<td>(fuel mass/dwell time)</td>
<td>A: 1mg-10mg / 400 μs dwell time</td>
</tr>
<tr>
<td></td>
<td>B: 1mg-1mg / 100 μs dwell time</td>
</tr>
</tbody>
</table>

Figure 2.3 shows the simulation results of each 2-D RIF model using injection strategy A. Since the oxygen concentration is 13% which is considered to be in a low temperature combustion regime, the auto-ignition of the fuel occurs at 1150 μs which is relatively slow due to the diluted mixture condition even though the mixture field from each injection event starts to interact at 735 μs. The criteria of whether the
mixture field is interacted can be determined by introducing the interaction factor I, which will be discussed in the next section.

While the flame structure looks similar in the beginning of the auto-ignition, the modified 2-D RIF model predicts the overall temperature of flame surface much smaller than the others. This is because the modified 2-D RIF model assumes the flame propagation from the first fuel stream to second fuel stream by replacing the solution of first fuel stream when the temperature reaches 2000K at the boundary of stoichiometric region (i.e. $Z=0.033$, $Z=0.08$). However, the maximum temperature cannot exceed 2000K under conditions of low ambient temperature and high EGR rate, which means that the assumptions of modified 2-D RIF model does not pertain, as mentioned earlier.

On the other hand, new simplification method is based on the relative proportion of the temperature at $y=0$, it is robust in terms of various ambient conditions. This can be also found in the 2-D temperature contour of figure 2.4 which represent the instantaneous solution of 2-D RIF model. The high temperature region propagates from $y=0$ to $y=1$ which means the mass and heat transfer from the first fuel stream to second fuel stream, and the maximum temperature always occurs at the stoichiometric mixture fraction. At 1250 μs when the discrepancies begin to appear, one can see that the modified 2-D RIF model cannot describe the appropriate auto-ignition of rich and lean region from $y=0$ to $y=1$ because the solution of rich and lean region is not replaced by that of $y=0$ in some region. Thus a particular temperature should not be a criterion of the solution replacement because the solution of rich and lean region may not be replaced after sufficient time, as shown in the contour of modified 2-D RIF model at 1500 μs of figure 2.4.
Figure 2.3. Calculated flame structure using each 2-D RIF model under injection strategy A (Full: original 2-D RIF model, Modified: 2-D RIF model with previous assumption, Present: 2-D RIF model with new assumption).
Figure 2.4. Instantaneous 2-D temperature contour of using each RIF model at ASOI 1250, 1350, 1400 and 1500 μs.
As mentioned before, previous assumption is not valid under the small amount of fuel injection with short dwell time which is a similar condition with two pilot injection under engine operating condition, and the difference between each 2-D RIF model is verified under the injection strategy B in table 2.2. The injection mass and dwell time has been reduced from the injection strategy A while the other conditions remain same.

Figure 2.5 shows the calculated flame structure of each 2-D RIF model at 950, 985, 1125, 1170 and 1225 μs ASOI. Unlike the injection strategy A, the auto-ignition of the first fuel stream occurs at 950 μs which is a long time after the interaction starts (625 μs) because there is no sufficient time to auto-ignite due to shorter dwell time than the injection strategy A. Thus the auto-ignition of second injection immediately occurs by the mass and heat transfer from the first fuel stream within 100 μs which can be found that the high temperature region of second injected fuel arises around 27 mm from the nozzle at 1125 μs ASOI. The propagation of the auto-ignition from y=0 to y=1 in rich and lean region cannot be described by the previous assumption because it cannot predict that the enthalpy of first fuel stream is propagated simultaneously with the auto-ignition of first fuel stream as shown in the red dotted line of figure 2.5.

In conclusion, a criterion of the solution replacement should be revised to predict the various ambient condition and the solution of rich and lean region should be interpolated by the enthalpy of the first and second fuel stream to describe the auto-ignition propagation phenomena from the first fuel stream to second fuel stream as the dwell time and fuel mass change. Figures 2.3-2.5 show that the new assumption is congruent with the original 2-D RIF model on the variation of combustion phenomena under various conditions, and the computational time can be reduced to the 22% of original 2-D RIF model.
Figure 2.5. (a) Calculated flame structure using each 2-D RIF model under injection strategy B. (Abbreviation is same with figure 2.4) (b) CPU time of each 2-D RIF model.
2.2.4 Extension of 2-D RIF model for 4-5 pulse injection system

Another limitation of 2-D RIF model is that the model could solve only two fuel stream based on each mixture fraction $Z_1$ and $Z_2$, which cannot be applicable to the commercial diesel engine under 4-5 pulse injection system including pilot, main and post injection. To overcome this limitation, 2-D RIF model has been extended to describe the multi-fuel stream with more than 3-pulse injection [82]. The main idea is that the instantaneous solution of 2-D RIF equation reaches a steady-state after sufficient amount of time, and it can be assumed to be one-dimensional solution because it has similar value after the steady-state regarding to the y-direction even though the solution in each y-axis has a different history of scalar dissipation rate (figure 2.6). Thus the 2-D RIF solution can be collapsed to one dimensional solution as shown in equation (2.2.25) which enables the 2-D RIF model to describe the following injection. The collapse of the two-dimensional solution can continue for any number of injection if certain conditions are satisfied.

\[
Y_i(Z) = \frac{\int_V \rho \tilde{Z}_i dV}{\int_V \rho \left( \sum_{j=1}^{N} \tilde{Z}_j \right) dV} Y_i(Z = Z_1) + \frac{\int_V \rho \tilde{Z}_2 dV}{\int_V \rho \left( \sum_{j=1}^{N} \tilde{Z}_j \right) dV} Y_i(Z = Z_2)
\]

(2.2.25)
To specify the validity of the collapse method, it is important to understand the auto-ignition process of each injection under multiple injection strategies. Figure 2.7 shows the instantaneous temperature solution of each fuel stream regarding mixture fraction domain which was solved by the flamelet model in the simulation result of figure 2.4. In case of the first fuel stream, the auto-ignition process is similar with the conventional diffusion flame where the initial reactions are occurred at the slightly rich region and following reactions increases the temperature as well as the diffusion to both directions regarding mixture fractions as shown in the left graph of figure 2.7, and the first fuel stream starts to auto-ignite about 940 μs ASOI which is relatively prolonged because of the high EGR rate condition.

On the other hand, the auto-ignition of the second fuel stream is somewhat different from that of the previous injection. The most noticeable difference is that the time to reach the steady-state solution is much faster than three times, and it cannot be explained by the increase of the ambient temperature due to the auto-ignition of first fuel stream because they are not much increased at the time when the second fuel stream begins to auto-ignite (400 μs after the auto-ignition of first fuel stream). The
process of the increase of temperature is also different in the second fuel injection case where the temperature increases along the stoichiometric mixture fraction. Meanwhile, figure 2.4 shows that the propagation of mass and heat from the first fuel stream (i.e. \( y=0 \)) reaches the \( y=1 \) axis at 1340 \( \mu s \) which is a 400 \( \mu s \) after the auto-ignition of first fuel stream, and it is exactly consistent with the time when the auto-ignition of second fuel stream is occurred. Furthermore, it is much shorter than the characteristic time of the fuel chemistry under such a high EGR and low temperature condition. Thus the auto-ignition of second fuel injection is mainly caused by the mass and heat transfer from the previous injection, and it is always faster than that of previous injection because the propagation speed is much faster than that of chemistry itself, which was also investigated in previous researches [79].
Figure 2.7. Auto-ignition process of each fuel injection. (a) Temperature history of the 1st fuel stream (y=0) where legend of the graph means ASOI (μs). (b) Temperature history of the 2nd fuel stream (y=1) where the legend of the graph means the time after the auto-ignition of 1st fuel stream (940 μs).
As a result, it is concluded that the solution can be collapsed after the second injection because the solution at y=1 has already reached a steady-state in the injection strategy A. Furthermore, it can be guessed that the solution can be collapsed at any time after the end of injection when the large amount of fuel is supplied as a second injection because the propagation time is much shorter than the injection duration even under the highly diluted condition listed in table 2.2.

From the previous analysis on the auto-ignition process of each fuel injection, it is easy to quantify the time needed to collapse the 2-D RIF solution. As mentioned earlier, the most important premise of the collapse method is whether the solution of 2nd fuel stream (y=1) has reached its steady-state. Thus the duration of the second injection is important to determine whether the collapse of the solution is possible because it can be collapsed when the injection duration is sufficiently longer than the start of auto-ignition. In addition, injection mass is also important to determine the auto-ignition time of second fuel stream because the propagation speed to y=1 is closely dependent on the scalar dissipation rate at stoichiometric mixture fraction of second injection (i.e. $\chi_{st,2}$). Thus the applicability of the collapse method can be investigated by checking the duration and mass of the second injection, and the criteria of which the solution has reached a steady-state is defined by the difference of solution at each fuel stream, as shown in equation (2.2.26)

$$\left| \frac{T(Z, y=0) - T(Z, y=1)}{T(Z, y=0)} \right| < 0.01, \text{ where } 0 < Z < Z_{\alpha} + \Delta Z$$

Equation (2.2.26) is based on the difference of temperature solution at each fuel stream, and it is enough to collapse the solution when its absolute value is within 1% of the temperature at y=0. To ensure that the solution after the collapse is similar with previous one by aspect of temperature, pressure and emissions, $\Delta Z$ is chosen two
times the value of stoichiometric mixture fraction. Quantitative analysis on the validity of collapse method in engine conditions will be discussed in the chapter 4 because the mixture composition, turbulence and injection parameter allowed in the single cycle during engine operation is quite different to that of simple 3-D domain.

2.2.5 Summary of modelling strategy using the new 2-D RIF model

Based on the formulation of 2-D flamelet model, section 2.2.3-2.2.4 deals with the improvement on simplification to increase the computational efficiency of the 2-D RIF model and the possibility of expanding to the 4-5 pulse injection system. Figure 2.8 shows the overall schematic diagram of modelling strategy using the modified 2-D RIF model with introducing the collapse method in the quadruple injection system which is widely used in commercial diesel engine.

As shown in figure 2.8, conventional 1-D RIF model resolves the combustion process first because there is only one fuel stream. The solution domain are extended to two-dimensional when the second fuel is injected, and the variable $Z_2$ describes the second fuel stream. The modified 2-D RIF model is not solved immediately because each fuel stream is spatially separated without any interaction. Thus the species and temperature solution of 1-D flamelet equation at each boundary (i.e. $y=0$ and $y=1$) represent the auto-ignition of each fuel stream and they are linearly interpolated in the intermediate region (i.e. $0<y<1$) by equation 2.2.26.

$$Y_i(Z, y)|_{0<y<1} = (1-y)Y_i(Z, y = 0) + yY_i(Z, y = 1)$$

(2.2.26)

Meanwhile, a criterion for determining whether the fuel stream interacts was suggested by previous work [79], as shown in equation 2.2.27.
After each mixture field are considered to be interacted, 2-D RIF model is solved by using the new simplification method as depicted in figure 2.2, and the model solved the mass and heat transfer from first fuel stream to second fuel stream at each time. By the time when the third injection starts, instantaneous solution of 2-D RIF model is collapsed by equation (2.2.25) after confirming that it satisfies the equation (2.2.26) to minimize the error before and after the collapse. Once the criteria in equation (2.2.26) is satisfied, the solution can be collapsed at the following injections that the previous procedure is repeated.

Figure 2.8. Modelling strategy of modified 2-D RIF model for quadruple injection system.
2.3 Chemical reactions

2.3.1 Fuel chemistry

Normal heptane ($nC_7H_{16}$) was selected as the representative fuel for the combustion simulation, and the chemical mechanism consists of 59 species and 293 reactions where the toluene and its cross-reaction with normal heptane were subtracted from the original reduced mechanism [112]. The chemical reaction includes the NO$_2$ and poly-aromatic hydrocarbon (PAH) chemistry for the detailed prediction of NOx and soot emissions, and the mechanism showed good agreement with various experimental results such as shock tube, constant volume vessel and diesel engine.

2.3.2 NOx model

Modelling of NOx emission in engine combustion processes focuses on the thermal NOx which is produced by pyrolysis of nitrogen atom in the high temperature region, because the other types of NOx formation are not significant in the combustion of hydrocarbon fuel. The most well-known chemistry of thermal NOx formation is the extended Zeldovich mechanism [9, 113]

\[
\begin{align*}
N_2 + O & \leftrightarrow NO + N \\
N + O_2 & \leftrightarrow NO + O \\
N + OH & \leftrightarrow NO + H
\end{align*}
\]  

(2.3.1)

Since NOx emissions is a sum of NO and NO$_2$ emissions, it is important to consider the mechanism of NO$_2$ emissions because the relative ratio of NO$_2$ is not
negligible under a particular combustion system [114], and it is also related to the soot oxidation [115, 116]. The chemistry of the NO-NO₂ conversion is

\[
\begin{align*}
NO + HO₂ & \leftrightarrow NO₂ + OH \\
NO₂ + H & \leftrightarrow NO + OH \quad (2.3.2) \\
NO₂ + O & \leftrightarrow NO + O₂
\end{align*}
\]

In this study, a mechanism reduced from GRI-mech 3.0 [117, 118] including the reactions in (2.3.1-2.3.2) was used and implemented in the fuel mechanism, which consists of 4 species and 12 reactions.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>(A)</th>
<th>(b)</th>
<th>Activation energy ((Eₐ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(N + NO = N₂ + O)</td>
<td>3.50E+13</td>
<td>0</td>
<td>330</td>
</tr>
<tr>
<td>2</td>
<td>(N + O₂ = NO + O)</td>
<td>2.65E+12</td>
<td>0</td>
<td>6400</td>
</tr>
<tr>
<td>3</td>
<td>(N + OH = NO + H)</td>
<td>7.33E+13</td>
<td>0</td>
<td>1120</td>
</tr>
<tr>
<td>4</td>
<td>(N₂O + O = N₂ + O₂)</td>
<td>1.40E+12</td>
<td>0</td>
<td>10810</td>
</tr>
<tr>
<td>5</td>
<td>(N₂O + O = 2NO)</td>
<td>2.90E+13</td>
<td>0</td>
<td>23150</td>
</tr>
<tr>
<td>6</td>
<td>(N₂O + OH = N₂ + HO₂)</td>
<td>4.40E+14</td>
<td>0</td>
<td>18880</td>
</tr>
<tr>
<td>7</td>
<td>(N₂O + H = N₂ + OH)</td>
<td>2.00E+12</td>
<td>0</td>
<td>21060</td>
</tr>
<tr>
<td>8</td>
<td>(N₂O(+m) = N₂ + O(+m))</td>
<td>1.30E+11</td>
<td>0</td>
<td>59620</td>
</tr>
<tr>
<td>9</td>
<td>(NO + HO₂ = NO₂ + OH)</td>
<td>2.11E+12</td>
<td>0</td>
<td>-480</td>
</tr>
<tr>
<td>10</td>
<td>(NO + O + m = NO₂ + m)</td>
<td>1.06E+20</td>
<td>-1.41</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>(NO₂ + O = NO + O₂)</td>
<td>3.90E+12</td>
<td>0</td>
<td>-240</td>
</tr>
<tr>
<td>12</td>
<td>(NO₂ + H = NO + OH)</td>
<td>1.32E+14</td>
<td>0</td>
<td>360</td>
</tr>
</tbody>
</table>
2.3.3 Soot model

Semi-detailed soot model [96] is a practical approach to calculate the soot emissions in diesel engines, because the detailed soot model takes too much time. The longer duration of time is not suitable for the application of engine development process and the simple phenomenological model cannot predict the behavior of soot precursor where the soot emissions are totally dependent on the fuel species and simply modelled equation.

The model consists of 6 equations which are 4 equations for the soot production and 2 equations for the soot oxidation respectively. The mechanism used in section 2.3.1 describes the formation of soot precursor by PAH species with following pathways.

(1) PAH species considered: A₁ (benzene) to A₄ (pyrene)

(2) Initial aromatic ring formation from the propargyl radical (C₃H₃) to benzene

(3) Hydrogen abstraction and carbon addition (HACA) process to the higher PAH species (pyrene as the largest PAH species)

Once the PAH species is produced, the soot formation is initiated through the inception of the A₄ (pyrene), surface growth, and coagulation to the large soot particle are followed. Furthermore, PAH species directly participates in the surface growth and soot coagulation, as shown in figure 2.9. Mathematical description of the overall process is listed in table 2.4.
Figure 2.9. Schematic diagram of soot emissions model (reproduce from original figure [119]).
Table 2.4. Model equations and reaction coefficients of semi-detailed soot model by [96]

<table>
<thead>
<tr>
<th>No.</th>
<th>Phenomena</th>
<th>Equation</th>
<th>Reaction rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Soot inception</td>
<td>$C_{16}H_{10}(A_4) = 16C(s) + 5H_2$</td>
<td>$\dot{R}_1 = k_1[A_4], \quad k_1 = 2 \times 10^3 \ [s^{-1}]$</td>
</tr>
<tr>
<td>2</td>
<td>Surface growth through $C_2H_2$</td>
<td>$C(s) + C_2H_2 = 3C(s) + H_2$</td>
<td>$\dot{R}_2 = k_2[C_2H_2], \quad k_2 = 9 \times 10^4 \exp(-12,100/T) \cdot \sqrt{S} \ [s^{-1}]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$S = \pi d^2 \rho N \ [cm^{-1}], \quad d = \left(6 \rho Y_{C(s)} / \pi \rho C(s) N\right)^{1/3} \ [cm] $</td>
</tr>
<tr>
<td>3</td>
<td>Soot coagulation</td>
<td>$nC(s) = C(s,n)$</td>
<td>$\dot{R}<em>3 = k(T)\left(\rho Y</em>{C(s)} / M_{C(s)} N\right)^{1/6} [N]^{1/6}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$k(T) = 2C_a \left(6M_{C(s)} / \pi \rho C(s) \right)^{1/6} \left(6K_{inc}T / \rho C(s)\right)^{1/2} \ [particle / cm^3 s]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$K_{inc} = 1.38 \times 10^{-9}$ (Boltzmann constant [J/K])</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$C_a = 9$ (agglomeration constant)</td>
</tr>
<tr>
<td>4</td>
<td>Surface growth and coagulation through PAH</td>
<td>$C(s) + PAH_{k,j} = C(s+k) + 0.5jH_2$</td>
<td>$\dot{R}<em>4 = \gamma</em>{k,j} \beta_{k,j} [PAH_{k,j}] \cdot N$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\gamma_{k,j} = 0.3, \quad \beta_{k,j} = 2.2(\pi K_{inc}T / 2\mu_j)^{0.5} (d_p + d_{PAH})^2 \ [cm^3 / s]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$d_{PAH} = 2.416 \times 10^{-8} (2m_j / 3)^{0.5}$, $\mu_j$ : reduced mass</td>
</tr>
<tr>
<td>5</td>
<td>Soot oxidation by oxygen</td>
<td>$C(s) + 0.5O_2 = CO$</td>
<td>$\dot{R}<em>5 = 12 / M</em>{C(s)} \left(K_{sPA/O_2} \left(1 + K_{sPA/O_2} \right) \right) x + K_{sPA/O_2} \cdot (1-x) \cdot S \ [mol / cm^3 s]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Coefficients were referred by [99]</td>
</tr>
<tr>
<td>6</td>
<td>Soot oxidation by OH radical</td>
<td>$C(s) + OH = CO + 0.5H_2$</td>
<td>$\dot{R}<em>6 = 12\gamma</em>{OH} X_{OH} T^{-1/2} \cdot S \ [mol / cm^3 s], \quad \gamma_{OH} = 0.13$</td>
</tr>
</tbody>
</table>

Note: $Y_{C(s)}$: Soot mass fraction, $N$: Soot number density [particle/m^3], $M_{C(s)}$: Molecular weight of carbon (1 2 g/mol), $\rho_{C(s)}$: density of graphite (2 g/cm^3)
Based on the reaction constant listed in table 2.4, final soot mass fraction and number density can be calculated by equation (2.3.1). The source term of the soot particle mass in equation (2.3.1) includes a unit particle of the solid carbon which is denoted by \( C_{\text{s}} \) in table 2.4, even though it is difficult to be considered as soot particle. This is because the carbon particle in solid state is difficult to react except for the oxidation process by oxygen or OH radical, and the solid carbon which is formed through reactions 1, 2 and 4, is then turned into a soot particle by soot nucleation process, or is oxidized by oxygen or OH radicals. A previous research showed that the carbon can be reacted with other species such as \( \text{CO}_2, \text{H}_2\text{O} \) and \( \text{NO}_2 \) in lean conditions; however, it includes both chemical reactions with heat and mass transfer [98]. Meanwhile, the incipient soot particle size is assumed to be 1.28 nm of diameter which is approximately equivalent to 100 carbon atoms [120].

\[
\begin{align*}
\dot{S}_{\rho C_{\text{s}}} &= (16\dot{R}_1 + 2\dot{R}_2 + 6\dot{R}_4 - \dot{R}_5 - \dot{R}_6) \cdot M_{C_{\text{s}}} \\
\dot{S}_N &= (16\dot{R}_1 \cdot \frac{M_{C_{\text{s}}}}{M_{\text{Nucleus}}} - \dot{R}_3) \\
M_{\text{Nucleus}} &= \frac{\pi}{6} d_{\text{nucleus}}^3 \rho_{C_{\text{s}}}, d_{\text{nucleus}} = 1.28
\end{align*}
\] (2.3.1)

Where,  
\( \dot{S}_{\rho C_{\text{s}}} \): source term of soot mass density (g/cm\(^3\)-s)  
\( \dot{S}_N \): source term of soot number density (particle/cm\(^3\)-s)  
\( d_{\text{nucleus}} \): soot inception particle nucleus (nm)
2.4 Spray model

2.4.1 Lagrangian approaches for the modelling of liquid droplet

It is important to predict the behavior of liquid fuel spray because the spatial distribution of fuel spray significantly affects the combustion characteristics in direct-injected compression ignition engine. Unlike turbulent flow field, fuel spray is considered as a dispersed phase in the form of liquid droplet and is affected by the turbulence, which results in turbulent dispersion of liquid particle. The direct-injected fuel undergoes atomization, breakup and vaporization process [9] which are modelled by a group of discrete droplet particles.

The basic conservation equations of momentum of liquid droplet is an interaction of liquid particle and surrounding flow field, as shown in equation (2.4.1)

\[
m_d \frac{d u_d}{dt} = F_{dr} + F_p + F_{vm} + F_b
\]  

(2.4.1)

Where,  

- \( m_d \): mass of droplet (kg)  
- \( u_d \): droplet velocity (m/s)  
- \( F_{dr} \): drag force  
- \( F_p \): pressure force  
- \( F_{vm} \): virtual mass force  
- \( F_b \): body force

The right side of the equation (2.2.26) is a sum of external force which changes the momentum of liquid droplet. The drag force is a resistance force due to the difference between flow and droplet velocity and the pressure force is a hydrodynamic force due to pressure gradient. Virtual mass force is a force induced by the entrained
flow from liquid droplet, and the body force means the effect of gravity and acceleration. Each force can be described by equation (2.4.2).

\[
\begin{align*}
F_{dr} &= \frac{1}{2} C_d \rho A_d |u - u_d|(u - u_d) \\
F_p &= -V_d \nabla p \\
F_{am} &= -C_{am} \rho V_d \frac{d(u_d - u)}{dt} \\
F_b &= m_d \left[ g - \omega \times (\omega \times r) - 2(\omega \times u_d) \right]
\end{align*}
\] (2.4.2)

Where, 
- \( C_d \): drag coefficient \\
- \( u \): fluid velocity (m/s) \\
- \( A_d \): droplet cross-sectional area (m²) \\
- \( \rho \): density of fluid (kg/m³) \\
- \( V_d \): droplet volume (m³) \\
- \( \nabla p \): pressure gradient (N/m³) \\
- \( C_{am} \): virtual mass coefficient (0.5 in this study [121]) \\
- \( t \): time (s) \\
- \( g \): gravitational acceleration vector \\
- \( \omega \): angular velocity vector \\
- \( r \): distance vector to the axis of rotation

In the case of mass conservation, the evaporation and condensation of liquid droplet should be considered because of the multiphase condition, and they can be described by partial pressure of vapor and surrounding gaseous mixture [122, 123].

\[
\frac{dm_d}{dt} = -A_K \ln \frac{p_t - p_{v,\infty}}{p_t - p_{v,\infty}}
\] (2.4.3)
Where,  
\( m_d \): mass of droplet (kg)  
\( A_s \): droplet surface area (m²)  
\( K_g \): mass transfer coefficient  
\( \rho_g \): gas pressure (Pa)  
\( P_{vs} \): partial pressure of droplet surface (Pa)  
\( P_{v,\infty} \): partial pressure of droplet surroundings (Pa)

Meanwhile, the energy conservation of liquid phase is derived by considering the evaporative heat and heat transfer from droplet surface, and the heat transfer coefficient ‘h’ is used which was suggested by El Wakil et al [124].

\[
\begin{align*}
    m_d c_{p,d} \frac{dT_d}{dt} &= -A_s q_{d}^{\star} + h_{fg} \frac{dm_d}{dt} \\
    q_{d}^{\star} &= h(T_d - T)
\end{align*}
\]  

(2.4.4)

Where,  
\( c_{p,d} \): mass of droplet (kg)  
\( T_d \): droplet temperature (K)  
\( h_{fg} \): latent heat of vaporization (J/kg)  
\( q_{d}^{\star} \): heat flux on the droplet surface (W/m²)  
\( h \): heat transfer coefficient (J/m²-K-s)

### 2.4.2 Breakup and atomization model

As mentioned earlier, fuel spray is modelled by a group of liquid droplet and their motions are described by conservation equations. Since the mass and size of each individual droplet can be changed by interacting them with the flow field on the droplet surface, appropriate modelling on the breakup and atomization is essential until it becomes to the vapor phase.
As for the modelling of fuel breakup process, Reitz and Diwakar model [111] was used in this study where the breakup of the liquid droplet is occurred by the aerodynamic forces. The temporal change of the droplet diameter is described by the stable diameter and corresponding characteristic time,

\[
\frac{dD_d}{dt} = -\frac{(D_d - D_{d,\text{stable}})}{\tau_{\text{breakup}}}
\]  

(2.4.5)

Where, 
- \(D_d\) : instantaneous droplet diameter (m)  
- \(D_{d,\text{stable}}\) : stable droplet diameter within specific time (m)  
- \(\tau_{\text{breakup}}\) : characteristic time scale of breakup (s)  
- \(t\) : time (s)

The stable diameter and characteristic time scale were determined at each time step, and Weber number was used as the criterion of calculating the droplet instability because the model presumes the breakup process as an interaction between the momentum of droplet and surface tension. It can be divided into two breakup regimes depending on the range of Weber number: bag breakup and stripping breakup.

Bag breakup is occurred at relatively low range of Weber number, in which the surrounding pressure gradient distort the droplet and break off the child droplet when it overcomes the surface tension of original droplet. On the other hands, stripping breakup can be occurred at a large range of Weber number, in which liquid droplet can be stripped due to the shear force on the droplet surface. The stable droplet diameter and characteristic time scale of each breakup mode are described by equation (2.4.5-2.4.6), and the empirical coefficient is determined at the next section by comparing with experimental results.
\[ We = -\frac{\rho |u - u_d|^2 D_d}{\sigma_d} \geq C_{bag,1} \]
\[ \tau_{bag} = \frac{C_{bag,2} \rho_d^{0.5} D_d^{1.5}}{4\sigma_d^{0.5}} \]

Where, \( We \) : droplet Weber number
\( \sigma_d \) : droplet surface tension
\( \rho_d \) : density of droplet
\( \tau_{bag} \) : characteristic time scale of bag breakup
\( C_{bag,1} \) : model constant (empirical) for bag breakup

\[ -\frac{We}{\sqrt{Re_d}} \geq C_{stripping,1} \]
\[ \tau_{stripping} = 0.5C_{stripping,2} \left( \frac{\rho_d}{\rho} \right)^{0.5} \frac{D_d}{|u - u_d|} \]

Where, \( Re_d \) : droplet Reynolds number
\( \rho \) : density of the flow field
\( \tau_{stripping} \) : characteristic time scale of stripping breakup
\( C_{stripping,1} \) : model constant (empirical) for stripping breakup

In addition to breakup and atomization model, the initial velocity was calculated by the given fuel injection rate and nozzle hole diameter and the cone angle was measured by conducting the rig experiment under the free spray condition of the injector used in the engine experiments. Bai’s spray impingement model [125] was also implemented within the lagrangian framework to predict the droplet-wall interaction, and O’rourke model was applied to predict the inter-droplet collision [126].
2.4.2 Validation of spray model

In order to determine the empirical coefficient in equation (2.4.5-2.4.6) and verify the spray model used in this study, simulation results are compared with experimental data under a ‘spray A’ condition of Engine Combustion Network (ECN) [127]. In particular, Sauter Mean Diameter (SMD) is compared with experimental result under spray A condition because the coefficients of breakup model are related to the primary and secondary breakup which affects the droplet size distribution. Table 2.5 shows the experimental condition of spray A used in the validation which is a non-reacting spray without any oxygen content under cold ambient condition.

### Table 2.5. Simulation condition for the validation of spray model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh type</td>
<td>3-D box mesh (54mm x 54mm x 108mm)</td>
</tr>
<tr>
<td>Oxygen content</td>
<td>O₂ = 0 % (non-reacting condition)</td>
</tr>
<tr>
<td>Fuel type</td>
<td>Normal dodecane (nC₁₂H₂₆)</td>
</tr>
<tr>
<td>Fuel Temperature</td>
<td>363 K</td>
</tr>
<tr>
<td>Injection pressure</td>
<td>1500 bar</td>
</tr>
<tr>
<td>Number of holes</td>
<td>1 (single hole)</td>
</tr>
<tr>
<td>Injection duration</td>
<td>1.5ms</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>900 K</td>
</tr>
<tr>
<td>Ambient pressure</td>
<td>60 bar</td>
</tr>
<tr>
<td>Validation parameter</td>
<td>Liquid / vapor penetration length</td>
</tr>
<tr>
<td></td>
<td>Sauter mean diameter</td>
</tr>
</tbody>
</table>

Figure 2.10 shows the simulation results of SMD regarding the change of the model constant in the breakup model. The calculated average droplet size using the default model constant suggested by previous work [111] predicts large droplet
diameter, and the breakup constants $C_{b1}$ and $C_{s1}$ are needed to be modified. The experimental data was obtained from the previous work [128] based on X-ray scattering to measure the droplet size distribution, and the SMD was measured up to 12mm from the nozzle. The simulation results are compared with experimental data in the range of 6 mm to 12 mm because the droplet size distribution is significantly affected by the internal nozzle flow model and the mesh refinement near nozzle. The average droplet size reaches its stable diameter at 6 mm because the ambient pressure is much larger than the atmospheric condition, and the decrease of bag breakup constant $C_{b1}$ which promotes primary breakup near the nozzle where $C_{b1}=1$ is in good agreement with experimental results as shown in figure 2.10.

Based on the revised spray model, the penetration length of both liquid and vapor phase is compared with experimental results under high ambient temperature condition listed in table 2.5. Figure 2.11 shows the comparison of liquid and vapor penetration length regarding the ASOI time, and it shows that the spray model nicely predicts both liquid and penetration length of experimental results. Nonetheless, there is some discrepancy in the liquid penetration length; however, the final value is well matched with the experimental result when it reaches a stable value of liquid penetration length which is after 0.3 ms.
Figure 2.10. Sauter Mean Diameter (SMD, μm) of experimental data (black) and simulation (color, dash/solid) by changing the breakup model constant.

<table>
<thead>
<tr>
<th>Model constant</th>
<th>Variable</th>
<th>Value (Default)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bag breakup constant</td>
<td>$C_{b1}$</td>
<td>6</td>
</tr>
<tr>
<td>Bag breakup constant (time)</td>
<td>$C_{b2}$</td>
<td>$\pi$</td>
</tr>
<tr>
<td>Stripping breakup constant</td>
<td>$C_{s1}$</td>
<td>0.5</td>
</tr>
<tr>
<td>Stripping breakup constant (time)</td>
<td>$C_{s2}$</td>
<td>20</td>
</tr>
</tbody>
</table>
Figure 2.11. Vapor penetration length (upper) and liquid penetration length (lower) results of experiments (solid) and simulation (dash) regarding the time ASOI [ms].
Chapter 3. Experimental and computational setup

3.1 Experimental setup

3.1.1 Engine experimental apparatus and base operating conditions

A 1.6-liter four cylinder light-duty diesel engine was selected to validate the combustion model. The target engine was equipped with a turbocharger as well as a common-rail injection system with solenoid-type injector. The compression ratio is 16, and the detailed specifications of engine are described in table 3.1.

Table 3.1. Target engine specifications

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>77.2 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>84.5 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>140.0 mm</td>
</tr>
<tr>
<td>Engine displacement</td>
<td>1592 cc (396 cc/cylinder)</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16.0:1</td>
</tr>
<tr>
<td>Piston bowl shape</td>
<td>ω-type</td>
</tr>
<tr>
<td>IVO/IVC</td>
<td>aTDC 17CA/aBDC 14CA</td>
</tr>
<tr>
<td>EVO/EVC</td>
<td>bTDC 23CA/bTDC 20CA</td>
</tr>
<tr>
<td>Injection system</td>
<td>Common-rail system with solenoid injector</td>
</tr>
<tr>
<td>Spray angle</td>
<td>149°</td>
</tr>
<tr>
<td>Injector hole diameter</td>
<td>0.119 mm</td>
</tr>
<tr>
<td>Number of injector hole</td>
<td>8</td>
</tr>
</tbody>
</table>
Figure 3.1 shows the schematic diagram of the engine experimental setup. The engine was connected to a 340 kW AC dynamometer controlled by PUMA dynamometer controller, and it was operated under steady-state condition. The experimental data was measured at the furthest cylinder away from the intake supply where the temporal fluctuation of air and EGR mixture is affected less by the intake flow motion. The fuel and coolant temperature were kept constant by the controller, and the fuel mass was measured by fuel flow meter (AVL-533S). In case of exhaust gas measurement, the EGR rate at the inlet of intake port was measured by the exhaust gas analyzer (HORIBA MEXA-7100DEGR) together with NO, THC and CO emissions. Furthermore, the mass of soot emissions was measured by Smokemeter (AVL-415S) and the number density was also measured by fast engine particulate analyzer (DMS-500) to validate the soot model.

Total of 4 cases were selected as base operating conditions which are equivalent to those of commercial vehicles. Additionally, the four cases include various load, rpm and injection strategies to verify the robustness and reliability of the combustion and emissions model, as shown in table 3.2.
Figure 3.1. Schematic diagram of the engine experiment.
Table 3.2. Base operating conditions for the numerical simulation

<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1500</td>
<td>4</td>
<td>33</td>
<td>Triple Injection (PI/PI/MI)</td>
<td>590</td>
<td>1.67</td>
<td>1.11</td>
</tr>
<tr>
<td>2</td>
<td>1750</td>
<td>6</td>
<td>28.3</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>940</td>
<td>1.39</td>
<td>1.32</td>
</tr>
<tr>
<td>3</td>
<td>2000</td>
<td>8</td>
<td>24.8</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1100</td>
<td>1.3</td>
<td>1.56</td>
</tr>
<tr>
<td>4</td>
<td>2500</td>
<td>10</td>
<td>0</td>
<td>Triple Injection (PI/PI/MI)</td>
<td>1340</td>
<td>2.15</td>
<td>1.94</td>
</tr>
</tbody>
</table>

*PI: Pilot Injection, MI: Main injection, Po: Post injection
3.1.2 Rig experimental setup for measuring the fuel injection rate

The injection rate should be measured to validate the simulation model more accurately because it is strongly related to the combustion and emissions characteristics. Furthermore, the opening behavior of injector needle is quite sensitive to the injection strategies because the needle is not in position at the start of injection under the multiple injection strategies due to the motion of previous injection. Thus the additional experiments were conducted to measure the actual injection rate under the same condition with engine experiments.

Figure 3.2 shows the experimental setup for measuring the injection rate. The measuring instruments are based on the Bosch’s method [129] where the change of flow velocity induced by fuel injection leads a pressure wave to propagate, and it is linearly dependent on the acoustic impedance.

\[
\dot{q} = A \times u
\]
\[
dP = a \times \rho \times du
\]

(3.2.1)

Where,  
\( \dot{q} \) : volumetric flow rate of fuel [m³/s]  
\( A \) : flow rate [m²]  
\( u \) : flow velocity [m/s]  
\( \rho \) : fuel density [kg/m³]  
\( p \) : pressure [Pa]  
\( a \) : sound of speed in fluid [m/s]

Based on equation (3.2.1), the injection rate can be calculated by the pressure which is measured by using the piezo-electric pressure sensor (Kistler 6052A). The injector used in the measurement is the same as what is used in the engine experiments, and the injection pressure and current is input to the injector driver.
Figure 3.2. Experimental setup for measuring the injection rate.
Figure 3.3 shows the process to obtain an injection profile from given injection signal and pressure under case 1 of the base operating condition as an example. The most important consideration during the measurement is remembering to maintain a similar environment to the engine experiments because the behavior of the injector needle is highly affected by the back pressure caused by the high pressure environment in diesel engines. Thus the engine experiment was conducted first, and the back pressure was obtained from the in-cylinder pressure at each start of injection. The injector used in the measurement was an analogous specification with that used in engine experiments and the injection parameter such as injection signal, pressure, timing and energizing time. In the end, the actual injection rate was obtained from the preceding variables as an input which is shown in figure 3.3, and the measured injection rate was averaged over 10 injection cycles.

Figure 3.3. Experimental procedure of injection rate measurement.
After obtaining the raw injection rate data, additional manipulation is needed to remove the unrealistic behavior such as negative injection rate and oscillation. Then the final injection rate, which is planned to be used later for the numerical simulation can be obtained. As shown in figure 3.4, it shows less than 1% error with that measured in the engine experiments.

Figure 3.4. (a) Final injection rate (solid line) and raw injection rate data (dashed line) where injection pressure is 590 bar. (b) Injection mass measured in the engine experiments (black) and from rig test (red).
3.2 Computational setup

In this study, a commercial CFD code star-CD v4.22 was used to calculate the unsteady RANS equations for mass, momentum and enthalpy, and the 2-D RIF model was coupled with CFD code. To implement the combustion and emissions model to the commercial code, the enthalpy equation was revised by mapping the chemical species obtained from the 2-D RIF model. Thus the commercial code only solves the heat transfer to the wall and the heat loss due to the spray evaporation, while the soot mass and number density are directly solved at each location in the physical domain by the equation (2.3.1) based on the chemical species such as pyrene (A₄), hydroxyl radical (OH), oxygen (O₂), acetylene (C₂H₂) which was solved in the 2-D RIF model.

As for the numerical discretization, finite-volume equations based on the implicit methods for the temporal discretization, and the mass continuity is enforced by the pressure equation which is called a Pressure Implicit with Splitting of Operators (PISO) algorithm which consists of predictor and corrector stage [130]. A time step of 0.1 CA (1.1 × 10⁻⁵ s at 1500 rpm) was used during the compression stroke before the start of first injection, and 0.05CA (5.5 × 10⁻⁶ s at 1500 rpm) was used during the combustion process. Meanwhile, spatial discretization method is varied according to each variable. A multi-dimensional 2nd order accurate differencing scheme [131] is used to solve the momentum and turbulence parameter, while the temperature and mass are calculated by upwind differencing and central differencing scheme respectively.

A 1/8 sector mesh was used to perform the CFD simulations with cyclic boundary conditions because the geometry of combustion chamber in diesel engine can be considered to be a axisymmetric, and the computational mesh was generated by automatic mesh generation software es-ice toolkit (Siemens PLM, 2017). The number
of cell is approximately 50,000 at IVC and 10,000 at TDC where the average cell spacing is 1mm, as shown in figure 3.5.

Figure 3.5. Computational mesh used in the simulation. (a) Mesh at TDC (b) Mesh at IVC
Chapter 4. Simulation results for model validation

This chapter covers the validation results of combustion and emissions model by comparing the experimental data under base operating conditions as well as some parametric variations of the operating strategies such as EGR rate, boost pressure and injection parameter. In addition, the reduction mechanism of NOx and soot emissions is quantitatively investigated and validity of the collapse method in an engine condition is confirmed to apply to the various injection strategies for reducing the emissions while maintaining the fuel economy level.

4.1 Simulation results of base operating condition

Figure 4.1 shows the history of pressure and heat release rate from simulation and experimental results under base operating condition. The combustion model can accurately predict the auto-ignition of each injection and the pressure rise, and the combustion duration is also well matched with experimental results where the time of SOC at each injection is less than 1 CA error with experiments and the error of maximum pressure is less than 2% of the average with that of experiments, as shown in table 4.1.

Table 4.1. Error analysis of the combustion model at each condition

<table>
<thead>
<tr>
<th>Case</th>
<th>$P_{\text{end of compression}}$ [%]</th>
<th>$P_{\text{max}}$ [%]</th>
<th>CA50 [CA deg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.14</td>
<td>2.06</td>
<td>1.39</td>
</tr>
<tr>
<td>2</td>
<td>0.32</td>
<td>0.14</td>
<td>0.75</td>
</tr>
<tr>
<td>3</td>
<td>-0.57</td>
<td>2.27</td>
<td>0.60</td>
</tr>
<tr>
<td>4</td>
<td>-2.01</td>
<td>-0.06</td>
<td>0.05</td>
</tr>
</tbody>
</table>

*Above error is based on the experimental data
Figure 4.1. Calculation (solid line) and experiments (dashed line) under base operating condition.
4.1.1 Simulation results of NOx and soot emissions

Figure 4.2 shows the simulation results of NO and soot emissions under base operating conditions. The overall trend of NO emission has a good agreement with experimental results even though their absolute values have some discrepancies. The difference of simulation and experiment may be caused by the inaccurate prediction of oxygen radical in the fuel chemistry because it can affect the initial reaction of NO emission. On the other hand, the soot model underestimates the mass density as compared to the experimental data because the oxidation rate by OH radical was over-predicted. The soot oxidation rate through OH radicals has been modified in the model suggested by Vishwanathan et al. [120] from original model by Fenimore and Johns [100] where the oxidation constant was increased by a factor of 12 which is considered to be an empirical constant.

![Figure 4.2. Emissions results of calculated (dashed line) and experimental (solid) data. (a) NO emission [ppm] (b) Soot mass density [mg/m³]](image)
Since the modified oxidation constant makes more soot oxidation by OH which results in underestimation of soot emission like in figure 4.2(b), parametric study on the modifying factor of soot oxidation constant was conducted factor in the range between each conventional model [100, 101], as shown in equation (4.1).

\[
\dot{R}_{\text{OH \_oxidation}} = K \cdot C_{\text{OH,FJ}} \cdot \gamma_{\text{OH}} X_{\text{OH}} T^{-1/2} \cdot S \text{[mol / cm}^3\text{s]}, \quad C_{\text{OH,FJ}} = 10.5833
\]  
(4.1)

Figure 4.3 shows the effect of oxidation constant on soot mass density by changing the constant K of equation (4.1). As expected, maximum soot mass decreases as K increases and K=3 is the best value to match with experiments. The revised constant shows a good agreement with experimental data under various operating conditions, as shown in figure 4.3(c).
Figure 4.3. Simulation results of soot mass density \([\text{mg/m}^3]\) by changing the oxidation constant in soot model. (a) Soot mass density vs. crank angle (b) Final soot mass density (line: experiments, filled: simulation) (c) Final soot mass density of the base operating conditions when \(K=3\).
4.1.2 Comparison of new simplification method of 2-D RIF model

A new method to simplify the solution of rich and lean region is suggested in this study, and it was compared with the previous method and the original 2-D RIF model under box mesh described in chapter 2. Since the previous discussion on box mesh was only focused on the flame structure, the effect of the simplification method in 2-D RIF model is quantitatively discussed in terms of the feasibility to predict the combustion process in engine operating conditions. Three models listed in table 2.2 were used again to calculate the combustion and emissions under engine operating conditions, and the target operating condition is 1750 rpm and BMEP 6bar condition (case 2 in base operating conditions).

Figure 4.4 shows the pressure of the main injection calculated by using each 2-D RIF model. The modified 2-D RIF model shows a little increase in heat release rate during the main combustion as compared to the other model, and the collapse method cannot be applied because the solution has not reached a steady-state due to the incorrect assumption in lean and rich region which results in a sudden increase of heat release rate near aTDC 20 CA, as shown in figure 4.4(a). In addition, it affects the emissions characteristics where the NO emission is over-predicted while the formation of soot emission is under-predicted.

On the other hand, present 2-D RIF model shows similar trends of heat release rate and emissions with those of original 2-D RIF model even though there is some discrepancies in the heat release rate at the start of combustion. The present 2-D RIF model predicts larger NO emission than the original model, which is a main reason of discrepancies in NO emission results of figure 4.2.
Figure 4.4. Simulation results of each 2-D RIF model (a) Heat release rate  
(b) Soot mass density [mg/m$^3$]  (c) NO emission [ppm].
4.1.3 Quantitative investigation of the multiple use of collapse method

The current study introduced the collapse method to mimic the multiple fuel stream with more than 3, and the quantitative analysis on the collapse method is needed to use the collapse method several times. In order to apply the collapse method, the instantaneous solution of the second fuel stream (i.e. \( y=1 \)) should reach near steady-state before the following injection event starts. Thus the time required for the solution of the second fuel stream to reach the steady-state (denoted by \( t_{st} \)) is compared with the corresponding injection duration (denoted by \( t_{inj} \)) and dwell time (denoted by \( t_{dt} \)) under each base operating condition, as shown in figure 4.5.

![Solution of 2nd fuel stream (y=1) reaches a steady-state.](image)

**Figure 4.5.** Definition of each time to ensure the validity of the collapse method under triple injection strategy.

In figure 4.6, all the times defined in figure 4.5 are compared for each injection strategy under base operating conditions. In case of injection strategy including pilot-main injection, time needed to reach the steady-state is always shorter than the
injection duration because the main injection duration is long enough for the solution of second fuel stream to reach the steady-state. Thus the collapse method can be applied at any time after the end of main injection under all the base operating conditions. On the other hand, it is possible that \( t_{st} \) is not shorter than \( t_{inj} \) because the injection duration is too short if the second injection is a kind of pilot injection. However, since \( t_{st} \) is shorter than the sum of injection duration (\( t_{inj} \)) and the dwell time (\( t_{dt} \)), there is no problem to apply the collapse method under the various operating conditions of the target engine, as shown in figure 4.6(b).

![Pilot-Main Case](image)

(a)

![Pilot-Pilot Case](image)

(b)

Figure 4.6. Comparison of each time (\( t_{st} \), \( t_{inj} \) and \( t_{inj}+t_{dt} \)) for each injection strategy under base operating conditions. (a) Pilot-main injections. (b) Pilot-pilot injections.
The results of figure 4.6 also show that the collapse method cannot be applied under certain conditions when the third injection is occurred before the solution of second fuel stream reaches a steady-state. There are two main possibilities for this:

(1) Auto-ignition itself is too slow due to the low ambient conditions such as high EGR rate

(2) Dwell time between 2\textsuperscript{nd} injection and 3\textsuperscript{rd} injection is too short to be nearly 100 μs

The first condition is usually the case when both pilot fuels are injected very early, such as low temperature combustion regime. In such a case, the application of the collapse method without solution reaching steady-state results in no significant error because the auto-ignition does not occur at both fuel streams. Figure 4.7 shows an example of the profiles of major species regarding the mixture fraction Z at bTDC 20 CA under low temperature combustion regime. It can be found that the maximum value of OH radical is similar in both fuel streams which means that the auto-ignition process occurs similarly in each fuel stream. Although the difference appears to be large in the figure 4.7(b) and 4.7(d), the absolute values of PAH and NO species in each fuel stream are not large because the auto-ignition has just started. On the contrary, the collapse method cannot be applied to the second case where the dwell time between each injection is extremely short, and the solutions to this limitation will be in the future works.
Figure 4.7. Solutions of the combustion species and emissions radicals at each fuel stream. (a-b) Profiles of the 1st fuel stream. (c-d) Profiles of the 2nd fuel stream. The engine operating condition is 1750 rpm and 6 bar with 40% of EGR rate, and the injection timings are bTDC 40 CA for 1st injection and 30 CA for 2nd injection, respectively.
4.2 Numerical evaluation of the combustion model

In order to ensure the applicability of the combustion model, the effect of grid size of the model is numerically investigated and compared with the results of using the ECFM-3Z model which is generally used in the numerical simulation in Diesel engines.

4.2.1 Effect of grid size on the combustion model

Unlike 1-D RIF model, the 2-D RIF model has two-dimensional solution domain which consists of $Z$ and $y$, and the $Z$ means the total mixture fraction which describes the composition of air and fuel mixture while the $y$ means the relative ratio of mixture fraction of each fuel stream and indicates which fuel stream is more dominant, as shown in figure 4.8.

Figure 4.8. Numerical grid of the solution domain in the 1-D RIF model (left) and 2-D RIF model (right).
Table 4.2 shows the simulation conditions regarding the grid size of the combustion model. The grid size is changed for both $Z$ and $y$ directions based on those used in previous simulations of base operating conditions, and the operating condition is chosen as 1750 rpm and 6 bar.

Figure 4.9 shows the simulation results of the heat release rate and the CPU time as the grid sizes for both directions change. For the direction of total mixture fraction $Z$, reducing the grid size does not significantly change the calculation result of heat release rate but; rather increases the CPU time, as shown in figure 4.9(a). The model predicts the auto-ignition faster when the grid size is increased because the coarse grid cannot accurately predict the auto-ignition process near the stoichiometric region. Thus the base grid sizes used in chapter 4.1 are optimal for the CPU time and the model accuracy. Meanwhile, changing the grid size regarding the $y$-direction mainly affects the auto-ignition of the main spray because the direction of $y$-axis is closely related to mass and heat transfer between each fuel stream. In this case, reducing the grid size over-predicts the propagation process from the first fuel stream to the second fuel stream due to the coarse grid. In addition, the increase of the heat release at an initial stage of the combustion of main fuel spray reduces the peak value of main heat release rate, as shown in figure 4.9(b). Nonetheless, the grid size of the $y$-axis is considered to be reasonable because the model is matched with experimental data within allowable error limit as mentioned in table 4.1.

<table>
<thead>
<tr>
<th>Operating condition</th>
<th>1750 rpm and 6bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size, $\Delta Z$</td>
<td>Base, 50%, 70%, 200%</td>
</tr>
<tr>
<td>Grid size, $\Delta y$</td>
<td>Base, 50%, 200%</td>
</tr>
<tr>
<td>Other simulation conditions</td>
<td>Remains constant</td>
</tr>
</tbody>
</table>

*Base grid size is same as the size used in the previous simulation (chapter 4.1).*
Figure 4.9. (a) Heat release rate history (left) and corresponding CPU time (right) as the grid size $\Delta Z$ changes. (b) Heat release rate history (left) and corresponding CPU time (right) as the grid size $\Delta y$ changes.
4.2.2 Comparison with ECFM-3Z combustion model

In this section, the combustion model developed in this study is compared with ECFM-3Z model to determine the model’s superiority. ECFM-3Z model solves the auto-ignition of chemical species along with the spatial mixing effect [72], and the CPU time drastically increases as the size of the chemistry to be considered in the calculation as well as the number of computational grid. The simulation is carried out under the base operating conditions of chapter 4.1 while the combustion model and corresponding chemical reactions are changed as listed in table 4.3.

Figures 4.10 and 4.11 show the simulation results of pressure and heat release rate under each operating conditions. At low load condition with high EGR rate, ECFM-3Z model cannot mimic the auto-ignition of both pilot and main injection because the simple chemistry coupled in the ECFM-3Z model fails to predict the auto-ignition, as shown in figure 4.10. Even though the heat release rate during the main injection seems to be well matched with experiments at high load condition, the auto-ignition of pilot injections is still not described by the model, as shown in figure 4.11. As a result, the discrepancies between each model are mainly caused by the fuel chemistry, and this can be solved by applying more detailed chemistry. However, large chemistry cannot be applied to the ECFM-3Z model as well as the large number of computational grid due to the drastic increase in the CPU time because it solves the auto-ignition at each location.

Table 4.3. Simulation conditions for the effect of grid size of the combustion model

<table>
<thead>
<tr>
<th>Operating conditions</th>
<th>Base 4 operating conditions in table 3.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion model</td>
<td>2-D RIF model</td>
</tr>
<tr>
<td>Chemistry</td>
<td>59 species, 293 reactions</td>
</tr>
<tr>
<td></td>
<td>ECFM-3Z model</td>
</tr>
<tr>
<td></td>
<td>7 species equilibrium</td>
</tr>
</tbody>
</table>
Figure 4.10. Time history of the in-cylinder pressure and the heat release rate under low load condition. Experiments (solid black line), simulation with RIF model (short-dashes black line) and with ECFM-3Z (long-dashes red line). (a) 1500 rpm and 4bar. (b) 1750 rpm and 6 bar.
2000rpm, 8bar (EGR=14%)

Figure 4.11. Time history of the in-cylinder pressure and the heat release rate under high load condition. Experiments (solid black line), simulation with RIF model (short-dashes black line) and with ECFM-3Z (long-dashes red line). (a) 2000 rpm and 8bar. (b) 2500 rpm and 10 bar.
4.3 Simulation results of parametric variation

Based on the simulation results in chapter 4.1-4.2, additional simulations regarding parametric variations of the engine operating condition are conducted to verify the robustness of the combustion model more thoroughly. The changing parameter was selected as injection timing, pressure, EGR rate and boost pressure, which are almost all parameters controllable in the engine operation.

4.3.1 Injection timing and pressure

At first, the injection parameters such as injection timing and pressure were varied to investigate the accuracy of the model because it is important to apply for the optimization of the injection strategy. All injection timings including pilot, main and post injection were advanced or retarded by 4 CA on the basis of case 2 in the base operating condition, and two cases were tested for the change of the injection pressure by 200 bar, and it is increased only by 100 bar in the case 4 because of the limit on maximum injection pressure. The other conditions remain to be the same as the base operating conditions to investigate the effects caused by injection parameter, as listed in table 4.4.

Figures 4.12 and 4.13 show the simulation results according to the change of injection timing. The overall pressure and heat release rate are well matched with experimental results as the injection timing and pressure change, and the model can be interpreted to capture these trends. Figure 4.12(c) shows the effect of injection timing on NO and soot emissions, and both NO and soot emissions decrease as the injection timing is retarded. The NO emission is known to be significantly dependent on the combustion temperature and thus it decreases as the injection timing is retarded.
because the start of combustion of main injection is delayed and the slope of heat release rate becomes slower with lower ambient temperature at the start of auto-ignition, which makes the premixed combustion phase shortened. As a result, advanced MFB 50 timing increases the maximum temperature of the combustion chamber which increases the NO emission, as shown in figure 4.13(c) and 4.13(d). In case of soot emission, it is needed to investigate the effect of both production and oxidation where the soot emission is mainly produced at the fuel rich region with the temperature more than 1800 K [9] and then oxidized by OH radicals around the stoichiometric region of the diffusion flame. As the injection timing is advanced, the soot formation is increased by the sooty area due to large high temperature region even though the oxidation rate is also increased by OH radical as shown in figure 4.13(d).

Meanwhile, the injection pressure affects the duration of each injection which changes the overall rise rate of in-cylinder pressure and heat release rate. Simulation results of figures 4.14 and 4.15 show that they are clearly decreased in low injection pressure case because of longer duration with slow injector opening rate, and maximum pressure and heat release rate are decreased as well. Thus the change of injection pressure reduces the premixed combustion phase while increases the mixing controlled combustion phase, which increases the NO emission and reduces the soot emission as shown in figures 4.14 and 4.15. Since the injection pressure is changed by 100bar upward in case 4, there is a little change in both emissions from the base case as shown in figure 4.15. From above simulation results, it is concluded that the model is robust to the change of injection parameters and it still shows a trade-off relationship between NO and soot emissions.
Table 4.4. Simulation conditions for the change of injection timing and pressure

<table>
<thead>
<tr>
<th>Case name</th>
<th>RPM [rev/min]</th>
<th>Load [bar]</th>
<th>Injection Strategies*</th>
<th>Boost pressure [bar]</th>
<th>Injection pressure [bar]</th>
<th>Injection timing variation</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-I1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1.32</td>
<td>840</td>
<td>Δ=-4CA</td>
<td></td>
</tr>
<tr>
<td>2-I3</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1.32</td>
<td>840</td>
<td>Δ=-4CA</td>
<td></td>
</tr>
<tr>
<td>3-P1</td>
<td>2000</td>
<td>8</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1.56</td>
<td>Δ=-200 bar</td>
<td>Δ=+200 bar</td>
<td>-</td>
</tr>
<tr>
<td>3-P3</td>
<td>2000</td>
<td>8</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1.56</td>
<td>Δ=-200 bar</td>
<td>Δ=+200 bar</td>
<td>-</td>
</tr>
<tr>
<td>4-P1</td>
<td>2500</td>
<td>10</td>
<td>Triple Injection (PI/PI/MI)</td>
<td>1.94</td>
<td>Δ=-200 bar</td>
<td>Δ=+100 bar</td>
<td>-</td>
</tr>
<tr>
<td>4-P3</td>
<td>2500</td>
<td>10</td>
<td>Triple Injection (PI/PI/MI)</td>
<td>1.94</td>
<td>Δ=-200 bar</td>
<td>Δ=+100 bar</td>
<td>-</td>
</tr>
</tbody>
</table>

*PI: Pilot Injection, MI: Main injection, Po: Post injection
Figure 4.12. Simulation results of injection timing variation. (a) In-cylinder pressure history. (b) Heat release rate history. (c) NO (left, ppm) and soot emissions (right, mg/m³).
Figure 4.13. (a) Time history of NO emission calculated by 2-D RIF model [ppm]. (b) Time history of soot mass density [mg/m³]. (c) MFB 50 (CA aTDC) as the injection timing changes. (d) Maximum temperature at the crank angle of MFB 50 (left) and average temperature of the region where the equivalent ratio is larger than 2 (right).
Figure 4.14. Simulation results of injection pressure variation under case 3 (2000 rpm and 8 bar). (a) In-cylinder pressure history. (b) Heat release rate history. (c) NO (left, ppm) and soot emissions (right, mg/m³).
Figure 4.15. Simulation results of injection pressure variation under case 4 (2500 rpm and 10 bar). (a) In-cylinder pressure history. (b) Heat release rate history. (c) NO (left, ppm) and soot emissions (right, mg/m^3).
4.3.2. Boost pressure and EGR rate

This section covers the investigation of the effect of ambient conditions on combustion and emissions characteristics under multiple injection strategies such as boost pressure and EGR rate. The increase of boost pressure makes more fresh air to come into the cylinder which changes the average equivalent ratio, and the change of EGR rate affects the gas composition of the ambient mixture and in-cylinder temperature due to the hot EGR mixture. Thus the validation of combustion model regarding the change of these conditions can ensure the model’s robustness to the in-cylinder mixture conditions. A change has been made to reduce the EGR rate from the base condition (case 2) while the boost pressure is increased from the base condition (case 3), and the other operating conditions remain to be same as listed in table 4.5.

Figures 4.16 and 4.17 show the pressure, heat release rate and emissions results according to the change of boost pressure. The pressure at the end of compression was increased at the higher boost pressure, which makes the overall pressure curve becomes higher. On the other hand, heat release rate shows a little difference because the oxygen concentration does not vary. In fact, the change of average equivalent ratio cannot largely affect the auto-ignition under the multiple injection because it is affected by the energy transfer from the existing flame (see section 2.2.3) whereas the premixed combustion where the flame speed is dependent on the equivalent ratio. Thus the emissions trend regarding the boost pressure is not caused by the difference in combustion phase but the change of ambient condition, and both NO and soot emissions decrease as the boost pressure increases because of lean mixture condition, as shown in figure 4.17.
EGR mixture is a burned gas re-circulated from the previous cycle and it is supplied and mixed with fresh air at the intake manifold in order to reduce the NOx emissions by adding the dummy species (i.e. CO₂, N₂ etc.) which is not participated in the auto-ignition. The effect of changing EGR rate on engine-out emissions is quite clear where the NOx emission is decreased while the soot emission is increased because the additional EGR rate reduced the supply of the fresh air under same boost pressure and makes more rich mixture.

Figure 4.18 shows the simulation results regarding the change of EGR mixture. The overall pressure increases at low EGR rate because the mixture temperature is decreased by lower EGR rate where the heat losses to the cylinder all are reduced. In addition to this effect, the increase of the oxygen concentration makes the combustion duration more shortened with earlier timing which results the increase of NO emission with decrease of soot emission due to longer premixed combustion phase. The model does well capturing these trends as shown in figure 4.18. As the EGR rate decreases, the NO emission is clearly increased while the soot emission is decreased, and the model also captures these trends excellently as shown in figure 4.18(c). Figure 4.19 well supports these trends very that the NO emission is decreased by the lower combustion temperature due to additional CO₂ and H₂O while the soot emission is increased due to lower oxygen contents.
<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
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</thead>
<tbody>
<tr>
<td>3-B1</td>
<td>2000</td>
<td>8</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1100</td>
<td>Δ=+0.2 bar</td>
<td>0</td>
<td>Base condition: Case 3</td>
</tr>
<tr>
<td>3-B2</td>
<td>2000</td>
<td>8</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>1100</td>
<td>Δ=+0.4 bar</td>
<td>0</td>
<td>Base condition: Case 3</td>
</tr>
<tr>
<td>2-E1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>840</td>
<td>1.32</td>
<td>Δ=-8%</td>
<td>Base condition: Case 2</td>
</tr>
<tr>
<td>2-E2</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>840</td>
<td>1.32</td>
<td>Δ=-13%</td>
<td>Base condition: Case 2</td>
</tr>
</tbody>
</table>

*PI: Pilot Injection, MI: Main injection, Po: Post injection
Figure 4.16. Simulation results of boost pressure variation. (a) In-cylinder pressure history. (b) Heat release rate history. (c) NO (left, ppm) and soot emissions (right, mg/m$^3$).
Figure 4.17. (a) Combustion phase of each boost pressure condition (CA50). (b) Time history of the NO emission [ppm]. (c) Time history of the soot emission [mg/m³].
Figure 4.18. Simulation results of EGR rate variation. (a) In-cylinder pressure history. (b) Heat release rate history. (c) NO (left, ppm) and soot emissions (right, mg/m³).
Figure 4.19. (a) In-cylinder temperature distribution at aTDC 15 CA as the EGR rate increases. (b) In-cylinder distribution of the oxygen mass fraction at aTDC 15 CA as the EGR rate increases.
4.3.3. Dwell time between each injection event

Previous results showed that the 2-D RIF model with new simplification method does well predict the overall trends of pressure, heat release rate and even both NO and soot emissions under various operating conditions. Additionally, more specific investigation of the changes in the dwell time between each injection event is discussed in this section.

Table 4.6 shows the simulation condition of the changes in dwell time. The reference condition is case 2 of the base operating conditions where the engine speed is 1750 rpm and the load is 6 bar BMEP. There are four injection events in the reference condition, which consists of two pilot injections, main injection and a post injection, and the change of dwell time between each pilot injection is simulated first.
Table 4.6. Simulation conditions for the change of dwell time between each injection event.

<table>
<thead>
<tr>
<th>Case name</th>
<th>RPM [rev/min]</th>
<th>Load [bar]</th>
<th>Injection Strategies*</th>
<th>Injection timing [us]</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>P2-A1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=-400 μs - - -</td>
<td></td>
</tr>
<tr>
<td>P2-A2</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=-600 μs - - -</td>
<td>P2 changes while P1, main held constant</td>
</tr>
<tr>
<td>P2-A3</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=-1600 μs - - -</td>
<td></td>
</tr>
<tr>
<td>P2-R1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=+400 μs - - -</td>
<td></td>
</tr>
<tr>
<td>P2-R2</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=+600 μs - - -</td>
<td></td>
</tr>
<tr>
<td>P1-R1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=+600 μs Δ=+400 μs</td>
<td>P1 changes while Δ P2=+600μs</td>
</tr>
<tr>
<td>P1-R2</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=+600 μs Δ=+600 μs</td>
<td></td>
</tr>
<tr>
<td>P12-A1</td>
<td>1750</td>
<td>6</td>
<td>Quadruple Injection (PI/PI/MI/Po)</td>
<td>Δ=-600 μs Δ=-600 μs</td>
<td>P1, P2 changes</td>
</tr>
</tbody>
</table>

*Reference base operating condition: 1750 rpm, 6bar
Figure 4.20 shows the time history of the heat release rate near TDC crank angle as the dwell time between each pilot injection event changes, and the result of experiments and simulation is separately illustrated because it is difficult to figure out if both results are depicted in the same graph. As the dwell time between each pilot injection increases, the location of the heat release rate due to first pilot injection is also advanced with decrease in the maximum heat release rate because the increase of dwell time means that the first pilot injection is occurred earlier under lower ambient temperature and pressure. The calculation result shows the small heat release rate near bTDC 10 CA while it is not found in the experimental results, and it is because the chemical mechanism predict the auto-ignition faster. On the other hand, it is delayed as the dwell time decreases and finally combined with the heat release of the second injection.

The change of dwell time between each pilot injection affects to the heat release rate near TDC, however, it cannot much affect the NO level because the main injection remains the same, as shown in figure 4.21(a). Even though it influences the auto-ignition of main injection, overall combustion duration during the main injection is almost the same which means that the premixed combustion phase changed very little, as shown in figure 4.21(b).

On the other hand, soot emission is decreased as the dwell time increases. While the NO emission is mainly produced by the premixed combustion phase of main injection, soot emission is a result of production and oxidation which is affected by the spatial distribution of mixture fields. Figure 4.22 shows the mixture contour and the corresponding distribution of equivalent ratio of two dwell times which are 1600μs advanced and 400μs retarded, respectively. As the dwell time decreases, the first pilot injection resides in the cylinder much closer to that of second injection and the mixtures of pilot injection are closely resemble. Thus richer mixture fields are formed
due to the retarded injection of first pilot spray which causes the main injection spray to drag more fuels. This causes more rich mixture near the piston bowl which increases the soot emission, as shown in figure 4.23(a). It is also explained by the time history of heat release rate during the mixing controlled combustion phase where the heat release rate decreased much earlier as the dwell time increases because the overall combustion speed increases due to the large area of mixture field, as shown in figure 4.23(b).

Meanwhile, the effect of changes in the second pilot injection is also calculated and compared with experimental data, as shown in figure 4.24. The injection timing of the second pilot injection is retarded from the latest timing of first pilot injection (case P2-R2) and heat release rate of each pilot injection is divided as the second pilot injection is retarded, and the model does well predict this trend. The NO emission is not changed as the second pilot injection changes because the main injection is fixed while the soot emission decreases as the dwell time increases, which is similar with the trends of figure 4.21.
Figure 4.20. Heat release rate history regarding crank angle degree. (a) Experimental results. (b) Simulation results.
Figure 4.21. Effect of dwell time between each pilot injection on the emissions level (Experiments: black line with diamond marker, simulation: red line with triangle marker). (a) NO emission [ppm] (b) Heat release rate from aTDC 10 CA to 40 CA (left: experiment, right: simulation) (c) Soot mass density [mg/m$^3$].
Figure 4.22. Mixture contour of pilot injections at aTDC 10 CA for each dwell time (upper) and the spatial distribution of equivalent ratio under sectional view (lower)
Figure 4.23. (a) Spatial distribution of soot mass fraction at aTDC 20CA. (b) Time history of heat release rate during the mixing controlled phase at aTDC 16~25CA.
Figure 4.24. Comparison of the calculation (red line with triangle marker) and experimental results (black line with diamond marker). (a) Time history of heat release rate near TDC. (b) NO emission [ppm] (c) Soot mass density [mg/m³].
Chapter 5. Numerical investigation of advanced injection strategies

The combustion model developed in this study was validated with the experimental results under various engine operating conditions as well as the variations of operating parameters. Based on the previous simulation results in chapter 4, effects of advance injection strategies on both emissions and engine noise are numerically investigated.

5.1 Effect of injection rate shaping

The injection rate shaping technology is to change the instantaneous injection rate under same injection pressure by controlling the opening rate of injector needle. Thus the maximum injection rate remains similar at the same injection pressure, but the initial slope varies, as shown in figure 5.1.

Figure 5.1. Example of the instantaneous injection rate when the injection rate shaping is applied (Base operating condition: 2000 rpm and 8bar, fast: fast opening slope, slow: slow opening slope).
Figure 5.2. (a) Time history of in-cylinder pressure (solid) and heat release rate (dash) of each different opening rate (black: base, red: fast, blue: slow). (b) Time history of NO emission (left, ppm) and soot mass (right, mg/m³). (c) Final NO emission (red dashes line, ppm) and soot mass (black solid line, mg/m³) of each different opening rate.
Figure 5.2 shows the simulation result about the effect of injection rate shaping on the combustion and emissions. The combustion phase is advanced a little as the opening slope becomes fast because the injected fuel mass until the start of combustion is largest in the fast opening case which promotes the premixed combustion and impedes the mixing controlled combustion. In detail, fast needle opening allows more fuel to be injected into the combustion chamber with higher injection momentum which increases the premixed air-fuel region. By the time when the combustion of main spray starts, more large area of premixed mixture is prepared to auto-ignite simultaneously which increases the NO emission due to the larger the flame surface area in the combustion chamber, as shown in figure 5.3(a).

On the other hands, the soot emission decreases at the fast needle opening because the fuel has already been injected into the cylinder while the fuel is still injected at the slow opening case, as shown in figure 5.3(b). Thus the averaged equivalent ratio over the combustion chamber is lower than that of slow needle opening case which decreases the soot emission.

As a results, it is concluded that the NO and soot emissions are affected by the initial injection rate while they still have a trade-off relationship. However, it is allowed to change the instantaneous injection rate at the same injection pressure, and it is expected to have a positive effect on the emissions and performances when combined with other operating strategies depending on the operating conditions.
<Temperature distribution at aTDC 15 CA>

(a)

<Figure 5.3. (a) Spatial distribution of in-cylinder temperature at aTDC 15 CA for each needle opening case and the following mass % of flame surface area to the combustion chamber (red: fast, blue: slow). The area enclosed by dotted lines means the region where the temperature exceeds 2,000 K. (b) Contour of the equivalent ratio at aTDC 18 CA for each needle opening case and the following averaged value.>

(b)

<Figure 5.3. (a) Spatial distribution of in-cylinder temperature at aTDC 15 CA for each needle opening case and the following mass % of flame surface area to the combustion chamber (red: fast, blue: slow). The area enclosed by dotted lines means the region where the temperature exceeds 2,000 K. (b) Contour of the equivalent ratio at aTDC 18 CA for each needle opening case and the following averaged value.>
5.2 Close pilot injection prior to main injection

As mentioned earlier, the injection rate shaping strategy can have an additional effect on the emissions when it is combined with other operating strategy. An additional pilot injection between the second pilot injection and the main injection can reduce both pressure rise rate and NO emission. If the small amount of fuel is injected just before the main injection with slow needle opening, the auto-ignition of the third pilot injection causes the small amount of heat release near aTDC 5 CA while the heat release of main injection decreases as shown in figures 5.4(a) and 5.4(b). This is because the part of fuel mass of the main injection is injected at the third pilot injection, and it can reduce the maximum pressure rise rate which results in the decrease of noise and vibration.

Furthermore, an additional pilot injection lowers the combustion temperature even though the overall injection timings are advanced as compared with the slow needle opening case. This is because a more fuel is injected during the pilot injection stages which does not significantly raise the combustion temperature, and the flame temperature from the main injection spray is decreased, as shown in figure 5.5(a). Thus the final NO emission is further reduced than that of the slow needle opening, as shown in figure 5.5(b), and this result is consistent with that of section 4.2.3 where the NO emission is strongly dependent on the heat release rate of the main injection.

Since the effect of pilot injection which is injected close to the main injection may have different effects depending on the operating conditions, various effects of the additional pilot injection will be investigated in the future works by using the combustion model of this study.
Figure 5.4. (a) Injection profiles used in the simulation of applying additional pilot injection (Blue: slow needle opening, red: fast needle opening, orange: additional pilot injection with slow needle opening). (b) Time history of pressure and heat release rate of each injection strategy. (c) Maximum pressure rise rate of each injection strategy [bar/deg]. Base operating condition is 2000 rpm and 8 bar.
Figure 5.5. (a) Temperature distribution in the combustion chamber of each injection strategy at aTDC 7 CA and 15 CA, respectively. (b) Final NO emission of each injection strategy [ppm]. Case name is same as figure 5.4.
5.3 Effect of boot injection

A boot injection is another method to reduce the noise and NO emissions by reducing the injection rate at the start of injection [132, 133]. Thus the effects of boot injection on the noise and NO emissions are investigated by using the combustion model developed in this study. Figure 5.6(a) shows the injection profiles when applying the boot injection with different boot length, and the end of injection remains similar while the initial mass flow rate is changed. As the boot length increases, the start of combustion is advanced and the overall heat release rate becomes smooth which means that the maximum pressure rise rate is reduced, as shown in figures 5.6(b) and 5.6(c).

On the other hand, figure 5.7 shows that the NO emission is slightly increased as the boot length becomes longer, which disagrees with the previous results where the pressure rise rate is related with the NO emission level. This is because the combustion phase is advanced to the TDC due to the changes in the start of injection which increases the high temperature region. Therefore, it is appropriate to analyze the effect of boot injection with the help of experimental approaches for more detailed evaluations.
Figure 5.6. (a) Injection profiles of the different boot injections (Black: base, blue: short boot length, red: long boot length). (b) Time history of pressure and heat release rate of each case. (c) Maximum pressure rise rate [bar/deg]. Base operating condition is 2000 rpm and 8 bar.
Figure 5.7. Simulation result of the soot mass density (black line with triangle marker, mg/m³) and NO emission (red line with diamond marker, ppm) when applying the boot injections.
Chapter 6. Conclusions

This study focused on developing a three-dimensional combustion model to simulate the combustion and emissions phenomena under multiple injection strategies, and aims to develop a robust model with high computational efficiency and applicability for engine development process.

The combustion model was constructed by the flamelet approach which can decouple the chemical reaction from the turbulent flow field. In particular, 2-D RIF model was used to describe the multi-fuel stream where two mixture fractions are introduced. Based on the original 2-D RIF model, improvements on the original model have been made in both ways. Because the original model had a limitation on the computational time when it is applied to the engine development process, a modified 2-D RIF model was introduced where the solution process is simplified except near stoichiometric region. The assumptions in previous works have been limited to apply the engine condition; however, new assumptions were proposed by means of enthalpy interpolation of each fuel stream. The new simplification method has been confirmed to have a higher accuracy in terms of the combustion phase, auto-ignition and emissions level with reasonable CPU time. Moreover, some correlations were formulated into the new method to reproduce the integral length scale profile for a variety of conditions from the sensitivity analysis. Then, the governing equation of the 2-D flamelet model was derived by the two different mixtures, which cannot be applied to the injection strategies with more than three injection events. Thus the collapse method was introduced where the instantaneous two-dimensional solution is reduced to one-dimensional solution, and the basis for simulating further injections was provided by presenting a quantitative criteria of the solution collapse.
An engine experiment was conducted to verify the reliability of the developed model, and the validations were conducted in following three stages.

First, four base conditions were selected including the various operating points from low speed and load to high speed and load, and the simulation results showed that there was an error in the maximum in-cylinder pressure and combustion duration within 2% and 1CA, respectively. Although the NO level was calculated to be higher compared to the experimental results, the overall trends were well predicted. In the case of soot emission, it was found that the original semi-detailed model over-predicted the oxidation rate via OH radical, and the optimal coefficient was derived through sensitivity analysis.

Second, the characteristics of combustion and emissions were measured by changing the injection timing, pressure and intake air condition and the simulation results were compared with experimental data. The model has demonstrated that the variations in the in-cylinder pressure, heat release rate and emissions level were well captured, and it is concluded that the developed model has a strong robustness for various ambient conditions and injection rates.

Finally, in a slightly more specific manner, the calculations using the model were carried out by varying the dwell time between each injection and comparing it with experiments. As the dwell time between each pilot injection was increased, there was no significant change in the NO emission because it cannot affect the premixed combustion phase of the main injection but, the soot emission gradually decreased because the location of high temperature region by pilot injection can reduce the formation of soot emission. These trends were consistent with that measured in the experiments, and they were explained by the simulation results by showing that the
soot emission is dependent on the spatial distribution while the NO emission is closely related to the premixed combustion phase of the main injection.

Through the verification process of the above three phases, the model has been shown to be highly reliable, demonstrating the model’s ability to quantitatively analyze the tendency of combustion and emissions, which are difficult to figure out by the experimental approach.

Based on the validation results, a couple of advanced injection strategies to reduce the NOx and soot emissions were proposed that are difficult to conduct with experiments. First, the effect of injection rate shaping strategy on both emissions was investigated. As the initial opening rate of the injector needle becomes faster, the NO emission was increased because more premixed fuel and air mixture is formed which promotes the premixed combustion phase, while the soot emission was decreased due to the enhancement on the mixing of air and fuel. An additional pilot injection with the slow needle opening could further reduce the NO emission as well as the pressure rise rate because the additional fuel is injected during the pilot injection stage instead of main injection which is the main cause of NO emission. Furthermore, the boot injection strategy could significantly reduce the pressure rise rate by increasing the injection duration at an early stage of the injection; however, more detailed analysis with the experimental approach is needed because both emissions were also increased because the combustion phase could not be maintained consistently.

Nonetheless, it is concluded that the model can provide the quantitative analysis on the effect of numerous multiple injection strategies to the combustion and emissions characteristics, and the model developed in this study can be used to propose optimal injection strategies for various engine operating conditions, and
reduce the emissions level of commercial diesel engines without any additional hardware changes by presenting the direction of development on injection technology.
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국문 초록

전세계적으로 환경 문제에 대한 관심이 높아짐에 따라, 자동차에서 발생하는 배출가스에 대한 규제는 지속적으로 강화되고 있는 추세이다. 특히 최근 대두되고 있는 미세 먼지 문제와 함께 디젤 엔진에서 발생하고 있는 문제들은 더욱 낮은 배출물 수준을 갖는 디젤 엔진의 개발을 요구하고 있다. 하지만 디젤 엔진에서는 연료를 직접 분사하여 연소되는 에너지를 동력원으로 하기 때문에 균일하지 않은 혼합기에 의한 확산 연소의 형태로 연소가 진행되며, 이는 질소 산화물과 입자상 물질을 동시에 저감하기 어렵다는 한계를 지니고 있다. 그러나 디젤 엔진은 높은 열효율의 측면에서 가솔린 엔진에 비해 장점을 갖고 있기 때문에, 많은 선행 연구들은 질소산화물과 입자상 물질을 동시에 저감할 수 있는 새로운 연소 기술을 제안하였다.

다단 분사 전략은 이러한 대안 중의 하나로, 단일 사이클에서 실린더 내에 연료를 여러 번에 걸쳐 나누어 공급함으로써 엔진에서 발생하는 소음, 질소산화물 및 입자상 물질을 저감하는 방법이다. 특히 common-rail system의 개발은 디젤 엔진의 연료 분사 기술을 한 단계 진보시켰고 연료 분사기를 비롯한 분사 시스템 전반에 대한 기술이 날이 갈수록 향상되면서 더욱 더 높은 압력에서 정밀한 연료 분사의 제어가 가능해지고 있다. 따라서 과거에는 불가능했던 분사 전략들의 실현 가능성이 높아짐에 따라, 매기 배출물을 추가로 저감할 수 있는 최적의 분사 전략을 개발하는 것이 중요해졌다. 하지만 선행 개발 단계에서는 실험적 기법으로 접근하는 데 한계가 있기 때문에, 전산 유체 역학(CFD)을 이용한 수치 해석 모델을 이용한 분석이 시간과 비용 절감의 측면에서 큰 장점을 갖는다.
따라서 본 연구는 다단 분사 현상을 모사할 수 있는 3 차원 연소 모델을 개발하는 데 초점을 맞추었으며, 엔진 개발 프로세스에 적용할 수 있도록 높은 계산 효율을 가지면서도 다양한 조건의 연료 분사 형태를 높은 정확도로 모사할 수 있는 강건한 모델을 개발하는 것을 목표로 하였다. 연소 모델은 화학 반응을 유동장으로부터 분리가 가능한 flamelet 기법 중 다단 분사를 모사하기 위해 확장된 2 차원 flamelet 모델을 구성하였고, 이를 바탕으로 두 가지 측면에서 모델을 개선하였다.

먼저 기존의 모델은 계산 시간이 너무 오래 걸렸기 때문에 엔진 개발 과정에 적용하지 못하는 문제가 있었기 때문에 화학 반응이 주로 발생하는 지역을 제외한 나머지 영역은 합리적인 가정을 통해 근사한 수정된 2 차원 flamelet 모델을 사용하였다. 하지만 기존 연구들에서의 가정은 엔진 조건에 적용하기에는 많은 한계가 있었고, 엔진 연소 조건에 적용 가능한 새로운 가정을 제안하였다. 새롭게 제안된 방법은 기존 모델에 비해 자발화 시점, 연소 기간 및 이로 인한 배기 배출물 예측에 있어 높은 정확도를 가짐을 확인하였다. 두 번째로, 2 차원 flamelet 모델의 지배방정식은 두 개의 서로 다른 혼합기장을 가정하여 유도된 식이므로 연료 분사 횟수가 3 회 이상일 경우를 모사하지 못한다는 단점이 있다. 따라서 본 연구에서는 2 차원 해를 1 차원으로 축소시킬 수 있는 collapse method 을 도입하고, 이에 대한 정량적인 기준을 제시함으로써 더욱 더 많은 횟수의 분사 조건도 모사할 수 있는 근거를 마련하였다. 이와 함께, 개발된 모델은 다환 방향족 탄화수소(PAH)의 상세 화학 반응을 포함하는 semi-detailed soot 모델과 결합하여 soot 배출물을 모사하였다.

개발된 모델의 신뢰도를 검증하기 위해 엔진 실험을 진행하였고, 실험 및 검증은 크게 세 단계로 구분하여 수행하였다. 먼저 다양한 운전 영역을 포함할 수 있도록 저속, 저부하 조건부터 고속, 고부하 조건까지 다양한 운전 조건을 포함한 4 개의 기본 운전점을 선정하였다. 또한 높은
신뢰도를 확보하기 위해 리그 실험을 통해 직접 연료의 분산율을 측정하였으며, 해당 조건에 대해 연소 압력, 열 발생률 및 배기 배출물 수준을 비교하였다. 계산 결과, 연소 압력은 최대압력 2%, 연소율 평균 1 도 이내의 오차로 높은 정확도를 갖는 것을 확인할 수 있었으며, 일산화질소 배출물 수준은 모델의 가정으로 인해 실험치에 비해 높게 예측되는 경향을 보였으나 전반적인 경향을 잘 예측하는 것을 확인하였다.

입자상 물질의 경우 계산에 사용된 기존의 semi-detailed soot model 이 OH radical 에 의한 산화를 과도하게 예측하는 경향을 보임을 확인하였고, sensitivity analysis 를 통해 최적의 계수 값을 도출하여 예측 정확도를 높였다. 또한 모델에 새롭게 적용된 가정이 엔진 운전 조건에서 기존 modified model 에 비해 높은 정확도를 가짐을 확인함과 동시에, 3 단 이상의 다단 분사를 모사하기 위해 collapse method 을 여러 번 적용하기 위한 정량적인 기준도 마련하였다. 또한 기본 4 개의 운전점에서 사용 소프트웨어에서 자주 쓰이는 다른 연소모델과 본 모델을 비교함으로써 모델의 우수성을 확인할 수 있었다.

두 번째로 모델의 강건성을 확인하기 위해 기존 운전점에서 분사 시간과 분사 압력, 흡기 조건을 변화시켜 가며 연소 및 배기 배출물 특성을 측정하였고, 계산 결과를 실험 결과와 비교함으로써 검증을 진행하였다. 모델은 운전 전략의 변경에 따른 압력, 열 발생률 및 배출물 수준의 변화의 경향을 잘 추종하는 것을 확인하였고 이를 통해 개발된 연소 모델이 다양한 흡기 조건 및 분산율에 대해서도 강건성을 갖는다고 판단된다.

마지막으로, 조금 더 구체적으로 들어가서 다단 분사 시 각 분사 간의 시간을 변화 시켜 가며 계산을 진행하였고 이를 실험 결과와 비교하였다. 각 파일럿 분사 사이의 시간을 변화시켜 가며 계산한 결과 질소 산화물은 큰 변화가 없었으나 입자상 물질은 점점 감소하는 경향을 보였고, 이는 실험에서 측정된 경향과 일치함을 확인하였다. 또한 이는 주 분사가
변하지 않기 때문에 영향을 받지 않는 질소 산화물과는 달리 입자상 물질은 공간적인 분포에 따라서 생성 및 산화율이 달라지기 때문으로 계산 결과를 통해 확인할 수 있었다. 위의 세 단계의 검증 과정을 통해 모델이 높은 신뢰도를 갖는다는 것과 함께, 실험에서는 분석하기 어려운 연소 및 배기 배출물의 경향을 모델을 통해 정량적으로 분석할 수 있음을 확인하였다.

앞선 검증 과정을 바탕으로, 개발된 연소 모델을 적용하여 실험적으로 수행하기 어려운 다양한 분사 전략이 질소 산화물 및 입자상 물질에 미치는 영향을 수치적으로 파악하였다. 동일 분사 압력에서 순간적인 분사율을 제어함으로써 실험 내 연료의 분포를 변화시킬 수 있는 Injection rate shaping 전략은 본 연구의 주요한 일자리 수록 입자상 물질의 발생이 줄어드는 반면 일산화질소 발생은 증가하였고, 이는 실험적 경향과 잘 일치하였다. 특히 이 전략은 여전히 두 배출물을 동시에 저감하기는 못하자 다른 운전 전략과 결합하였을 때 높은 효과를 낼 수 있기 때문에, 주 분사 연료의 일부를 세 번째 파 일을 분사로 분리함으로써 압력 상승률 및 일산화질소 배출을 저감할 수 있는 가능성을 확인하였다. 한편, boot injection 전략 또한 분사 초기의 유량을 제어함으로써 압력 발생률을 획기적으로 감소시킬 수 있음을 확인하였다.

따라서 본 연구에서 개발된 모델은 목적에 맞는 다양한 분사 전략을 제안하는 데 활용될 수 있으며, 분사 기술의 개발 방향 또한 제시함으로써 추가적인 하드웨어 변경 없이 양상 디젤 엔진의 배출물 수준을 저감하는 데 활용할 수 있을 것으로 기대된다.

주요어: 디젤 엔진, CFD, 질소산화물, 입자상 물질, 2-D flamelet 모델, 다단 분사 전략, 선행 분사 전략
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