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PHYSICS-BASED MODELS FOR ENGINE SYSTEM STUDIES: QUASI-D DUAL-FUEL COMBUSTION AND REAL-TIME INTAKE CHARGE FLOW ESTIMATION

A Dissertation
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the Graduate School of
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In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Automotive Engineering

by
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Accepted by:
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Dr. Mark Hoffman
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ABSTRACT

Ever tightening emissions and fuel economy regulations provide a strong impetus for research on high-efficiency low-emission engine concepts. In addition, CO₂ emission regulation and energy security considerations motivate investigations focused on alternative fuels. In the current heavy-duty fleet, diesel engines dominate the market due to their unmatched thermal efficiency. Nevertheless, they suffer from NOx and soot emissions and require complex aftertreatment systems to meet stringent regulations. Due to recent advancements of the Natural Gas (NG) extraction technology, its supply has become increasingly abundant. Conversion of Heavy Duty engines to NG operation provides a most effective way of increasing utilization of this low-carbon fuel in transportation, and reducing its dependence on oil.

Dual-fuel engines currently offered by OEMs are invariable conversions to spark ignited (SI) combustion. The compression ratio (CR) is lowered compared to diesel, and the engine operates with stoichiometric mixture in order to enable application of a Three-Way Catalyst. Dual fuel NG-diesel engines offer an attractive alternative. NG is mixed with air in the intake system, and a relatively small amount of diesel fuel is injected directly into the cylinder to initiate combustion. In that case, the conversion from a conventional diesel engine requires little modification of engine hardware. High CR is retained, and the engine can operate lean; hence, there is a prospect of achieving roughly the same thermal efficiency as in the case of a diesel baseline. Range anxiety is avoided, since the truck can continue running solely on diesel fuel if NG filling station is not available.
Development of the dual-fuel concept requires systematic investigations of maximum substitution rates, while addressing challenges such as the combustion stability, knock, transient response and methane slip. Since combustion characteristics are not fully understood, and increased degree-of-freedom (DOF) in modern engines demand excessive calibration effort, traditional development process that relies on experimentation becomes very costly. A predictive engine-system simulation built around physics-based models can provide a paradigm shift, by enabling investigations of the design options and pre-development of the complex multi-variable control strategies on the computer. Extension of the physics-based approach can also yield very effective virtual sensing of intake charge flow, and support development of a next-generation transient air-to-fuel ratio control. Main contributions of this research are such models, namely (i) a hybrid diesel + NG dual-fuel combustion model, based on the multi-zonal diesel spray/combustion model and a turbulent flame propagation model of NG-air mixture, and (ii) a model of intake charge mass-flow rate that utilizes intake manifold pressure as a single pressure input, and simultaneously solves differential equations for gas flow and cylinder pressure.

Dual-fuel combustion model addresses two modes of combustion taking place simultaneously in the cylinder. Diesel fuel injection, spray penetration, droplet evaporation, mixing, autoignition, heat release and emission formation are captured with a multi-zonal model. Original correlations were developed for ignition delay predictions in a dual fuel engine, spray penetration with high injection pressure, and heat release in the presence of Exhaust Gas Recirculation (EGR). Combustion of diesel fuel provides
multiple ignition sites for the surrounding NG-air mixture. Initial flame kernels grow and merge to eventually form a flame front surrounding each of the sprays. An original model of the flame front geometry, and its interactions with surrounding flames and combustion chamber walls, is developed to provide foundation for application of the turbulent flame propagation model. Energy cascade approach is utilized for prediction of the time-based turbulent flow field characteristics, and a reduced chemical kinetics reaction mechanism is included for estimation of knock. Finally, sub-models are implemented in a Zero-D thermodynamic engine cycle simulation to create a predictive, and yet computationally efficient Quasi-D simulation tool.

Accurate fuel metering requires accurate estimation of the intake charge mass. A universal feedforward intake air charge mass estimation method that requires reduced calibration effort, and a minimal set of sensors is pursued in this research. Simultaneous integration of differential equations capturing the variations of mass flow rate and the cylinder pressure yields a *Single-pressure* algorithm. It is capable of converging on correct values for both the mass air flow and cylinder pressure, given the known pressure upstream of the valve. Thus, it eliminates the need for the Mass Air Flow meter, and enables robust control of Air-to-Fuel mixture under both steady and transient operating conditions.

Experiments in the engine test cell were utilized to aid model development and provide data for model validation. In case of the intake charge mass estimation, the newly developed *Single-pressure* model was implemented in the research-grade engine electronic control unit, to demonstrate its ability to provide accurate estimations over a
federal driving schedule using an engine-in-the loop transient testing capability. Finally, rigorous in-vehicle testing was pursued subsequently to further test the accuracy, fidelity and real-time performance of the model.
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CHAPTER ONE
INTRODUCTION

Background

Energy security concerns and greenhouse gas (GHG) effect have driven the government to tighten the fuel economy and CO₂ emission regulations on vehicles. US Environmental Protection Agency (EPA) and National Highway Traffic Safety Administration (NHTSA) has announced Tier 3 fuel economy regulations of 54.5MPG and GHG emissions of 163g/mi for combined car and light truck fleets by 2025 [1]. Stringent regulations provide strong impetus for automakers and researchers to develop and adopt new technologies on vehicles. Since the power plants on majority of vehicles are internal combustion engines (ICE), improving the efficiency and reducing tailpipe emissions are paramount. Currently, the ICEs in the US market are dominated by two types, namely spark ignited (SI) gasoline and compression ignited (CI) diesel engines, where SI engines hold a large market share in passenger cars while CI engines dominate the heavy duty (HD) sector.

Diesel engines dominate the HD market due to their intrinsically higher thermal efficiency which stems from unthrottled operation, high compression ratio (CR) and lean combustion. However, conventional diesel engines suffer from the tradeoff between the NOx and soot emissions. This necessitates after-treatment systems and increases complexity. While the diesel engine manufacturers continue to refine their products in response to the recently introduced CO₂ reduction regulations [2], the increased cost of
aftertreatment and energy security concerns on petroleum fuel reserves have provided incentives for engineers to consider alternative fuels. Recent advancements of the NG drilling technology have greatly increased the estimated US and global reserves. As a consequence, all forecasts indicate that the price will remain lower than diesel fuel for many years to come. As of year 2015, diesel price is $22.08/BTU while natural gas is only $9.97/BTU[3]. This stimulates increased focus on utilization of Natural Gas (NG) in the HD sector.

Dual-fuel engine is a relatively new concept compared to conventional SI gasoline and CI diesel engines. Dual-fuel engines are generally direct conversions from diesel engines, where NG is port fuel injected upstream of the intake and is ignited through the combustion of diesel pilot. Early researches of dual-fuel engines have revealed several problems such as knock and combustion instability [4-10]. A combination of the flame propagation through the NG-air mixture and a high CR brings a risk of knock, especially at high loads where NG substitution rates are elevated. At light load conditions, dual-fuel engines are subjected to combustion instability due to slow flame propagation in a very lean mixture. Possible cylinder-to-cylinder variations can exacerbate the instabilities. Incomplete combustion and flame quenching contribute to methane slip, a phenomenon of a great environmental concern as methane has as high as 34 times the greenhouse effect of CO₂ if climate-carbon feedbacks are included. [11]

More recent dual-fuel engine research efforts were focused on maximizing NG substitution rate. Specifically, range of dual-fuel operation is extended by avoiding knock at high loads and ensuring combustion stability at low loads. An advanced pilot injection
dual-fuel engine concept was proposed [12-18], which applies an advanced (~60 BTDC), small amount of diesel fuel injection as the ignition source, with the port fuel injected NG as the main heat release source. In this concept, the onset of combustion is predominately controlled by chemical reactions. The advanced diesel injection results in a long ignition delay and better charge mixing, thereby reducing the rich pockets of diesel fuel and minimizing soot emissions. The better mixing of diesel and surrounding air and NG mixture also helps the ignition of NG, resulting lower local temperatures and reducing NOx emissions.

However, the combustion characteristics of dual-fuel engines are not yet fully understood. In particular, combustion instability at low load along with methane slip in a dual-fuel engine remains a problem and. Additionally, most of existing work on dual-fuel engines focus on the operating conditions with high NG substitution rates where diesel fuel is only used as an ignition source. Few published studies have specifically addressed the conditions where diesel fuel is also a major source of energy release.

In the light duty sector, multiple new technologies are introduced to improve the efficiency of the SI engines, and facilitate low-emission control strategies. Among others, turbocharging, variable valve timing and lift, direct injection and cooled Exhaust Gas Recirculation (EGR) are applied to create a flexible, but also very complex engine system. This poses new challenges related to development of feed-forward control strategies, as well as their implementation to accurately control the mixture composition under transient operating conditions. Traditional methods based on the application of a Mass Air Flow (MAF) meter or a speed-density approach are challenged, and fresh ideas
are sought to provide accurate and robust techniques for real-time estimation, while avoiding increased application of costly physical sensors, e.g. cylinder pressure transducers.

**Motivation and Scope**

Typical approaches to develop an ICE generally require extensive experimental implementations and testing. Experimental study is the ultimate way to validate a concept and provide insight into the development process. However, experimental implementations are associated with high time and financial costs. Availability of hardware imposes very hard constrains. Additionally, experimental data does not always reveal the underlying mechanism of the observed phenomenon and some information such as instant in-cylinder gas temperature and compositions are very hard to measure.

On the other hand, a predictive engine cycle simulation enables investigation of a broader operating space and efficient optimization of the engine calibration. Engine system configurations and advanced strategies can be investigated prior to fabrication of prototype parts. Even when in-depth experimental data are available, the simulation can complement the results by providing values of parameters that cannot be easily measured.

A cycle simulation of an engine system contains two major elements: gas exchange and combustion processes. The gas exchange process determines the mass and composition of the in cylinder gas when intake valve is closed. The compression/combustion process determines the reactions and the change of in cylinder gas properties between the intake valve closing and exhaust valve opening. A predictive cycle simulation of a dual-fuel engine will be invaluable for detailed characterization of
diesel-NG fuel injection strategies, optimal substitution rates and knock or stability limits. Additionally, predictive gas exchange and combustion models with reasonable calculation requirement is key enabler for accurate control of Air-to-Fuel Ratio (AFR), particularly under transient conditions.

From a control perspective, physics based models are universally applicable, and are possibly more accurate. It is also a much better option for developing a control oriented model, compared to empirical models.

Generally, the selection of modeling approach is based on application requirements. As shown in Figure 1.1, computing load increases exponentially with model fidelity and predictiveness. Thus a trade-off exists between computational cost and model fidelity.

![Figure 1.1 An illustration of trade-off between computational cost, spatial resolution and model fidelity](image)

In this study, the model for air charge mass flow prediction is designed for real-time vehicle on-board applications, where computation effort is a key factor. Hence,
Zero-Dimensional (Zero-D) modeling approach is selected. On the other hand, a predictive combustion model for a dual-fuel engine requires spatial resolution for adequate fidelity and predictiveness, but the model should also retain the computational efficiency. Thus Quasi-Dimensional (Quasi-D) modeling is selected as the approach for combustion modeling.

Figure 1.2 shows a summary for the scope of this work. The plot shows a schematic description of the intake air path and the cylinder of an Internal Combustion Engine. The scope involves modeling the intake air charge mass flow at the location of intake valve, from intake valve opening (IVO) to intake valve closing (IVC), and modeling of the combustion process in the cylinder from intake valve closing (IVC) to exhaust valve opening (EVO). The engine types considered include SI gasoline engines, CI diesel engines and CI dual fuel engines. The main contributions from this work include the following:

- Development of a universal Zero-D crank-angle resolved air charge mass prediction model, suitable for real time application in a high-degree of freedom engine, with a reduced set of sensors.

- Development of a Quasi-D model for dual-fuel engines, based on the multi-zonal diesel spray/combustion model and a model of turbulent flame propagation in NG-air mixture surrounding the spray.

A review of dual-fuel engines and previous work by others is given in Chapter 2. A Zero-D modeling and analysis of a dual-fuel engine is discussed in Chapter 3, followed by the development and validation of a Quasi-D multi-zone combustion model for diesel...
engines in Chapter 4. A detailed discussion of Quasi-D modeling of dual-fuel combustion is provided in Chapters 5 and 6. The development and validation of the air charge prediction model are discussed in Chapter 7. Summary of contributions and outlook are given in the closing Chapter.

![Diagram of modeling approaches and scope of work]

**Figure 1.2 Illustration of the scope of work and the modeling approaches.**

**Objectives**

The high-level objective is to develop a zero-D/Quasi-D modeling platform for ICEs with enhanced predictiveness of the intake and combustion process models. In particular, original contributions are needed in order to enable development of a fully predictive model of dual-fuel combustion, where the mixing-controlled combustion of
diesel fuel progresses in parallel with turbulent flame entrainment of the NG-air mixture. In case of the gas exchange modeling, main research driver is the need for a universal, physics based model for real-time estimation of the intake charge flow in an engine with an arbitrary set of actuators (e.g. VVT, VVA etc.), without the need for a Mass Air Flow meter, nor an extensive set of experimentally generated look-up tables.

Detailed objectives are summarized as follows:

**Quasi-D Dual-Fuel Combustion Model**

The dual-fuel engine studied in this work is a conversion from a conventional diesel engine, thus some characteristics of diesel engines are maintained, while the inclusion of an additional gaseous fuel increases complexity of the combustion process. The objective is to develop a multi-zone Quasi-D predictive combustion model for dual-fuel combustion, where the combustion modes of both fuels are to be captured simultaneously. A combination of multi-zonal approach and turbulent flame entrainment will be considered, to ensure required fidelity without the need for detailed spatial resolution provided by computationally intensive CFD simulations [17-24].

Combustion of diesel fuel is a mixing-controlled process, as postulated by Dec [25], while oxidation of NG premixed with air occurs in the turbulent flame front. The model should have the fidelity to predict the heat release contribution from each fuel, but carry out calculations simultaneously, and capture the interactions between the two. More specifically, autoignition of diesel fuel at multiple locations will provide ignition sites for NG/Air mixture, while presence of NG in the intake charge affects the ignition delay of diesel. A particular challenge is modeling of the flame front geometry, and its
interactions with other flame fronts surrounding adjacent sprays and the combustion chamber walls. The behavior of diesel spray, propagation of NG flame, in cylinder gas composition and properties, rates of heat release, and NOx formation are the outputs of the model.

To realize these objectives, several challenges need to be addressed: 1). Capturing two modes of combustion in a common space, namely premixed & mixing controlled burning of diesel fuel, and turbulent flame propagation of NG-air mixture. 2) Modeling the spray-combustion phenomenon of diesel fuel. The combustion of diesel fuel is a mixing-controlled process and requires careful attention to capture the spray breakup, evaporation, fresh charge entrainment and heat release in the chamber filled with NG-air mixture. 3). The flame propagation of NG-air mixture. The combustion of NG is initiated by the burning of diesel fuel, where multiple ignition sites form a flame front that propagates to the end gas zone. One of the key challenges in this work is to model the evolving flame front and its interaction with boundaries.

Crank-Angle Resolved Air Charge Mass Prediction Model

The second objective of this dissertation is to develop a universal air charge estimation approach which requires little or no calibration effort, while maintaining high prediction accuracy under both steady-state and transient conditions. The model outputs crank-angle resolved information about flow and composition at the intake valve during the intake process. Due to its physics-based nature, the model can be a universal solution for various engine platforms, and it requires a reduced set of sensors.
Several challenges are associated with this task, namely: 1) Realizing crank-angle resolved air charge prediction at the location of intake valve requires pressures upstream and downstream as inputs. However, pressure transducers with fast sampling rate are too expensive for production car applications. 2) Physics based models require significantly more computational effort than lookup based models. The model need to be simple for real-time execution, while maintaining the required fidelity and predictiveness. 3) The model needs to be reliable and robust; therefore, the model sensitivity to inputs and sources of error need to be carefully addressed. 4) The model is expected to provide a universal solution for various engine platforms, which is an additional challenge in designing the algorithm.

In summary, a key objective is to develop a physics based model for compressible gas flow across the valves, capable of real-time predictions for control of Air-to-Fuel ratio during steady or transient operation, while not requiring an additional cylinder pressure sensor, nor a Mass Air Flow meter.

Literature reviews for the dual-fuel modeling work and the intake charge mass estimation are presented separately, in Chapter 2 and 7, respectively.
CHAPTER TWO
DUAL-FUEL ENGINES: A REVIEW

Introduction

An emerging market trend stimulates increased focus on Natural Gas (NG) utilization in the HD sector. Recent advancements of the NG drilling technology have greatly increased the estimated US and global reserves [26] which is also demonstrated in the trend shown in Figure 2.1. As a consequence, all forecasts indicate that the price will remain roughly $2 lower on the diesel fuel gallon equivalent basis for many years to come. Figure 2.2 gives a comparison of fuel prices between diesel and NG in the last 14 years. It is clear that NG has a great advantage over petroleum fuel in terms of cost.

Figure 2.1. World NG production from 1988 to 2013 [27]
Table 2.1. Typical composition of NG [28]

<table>
<thead>
<tr>
<th>Composition</th>
<th>Content (%)</th>
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<tbody>
<tr>
<td>Methane</td>
<td>92</td>
</tr>
<tr>
<td>Ethane</td>
<td>3.2</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>3.0</td>
</tr>
<tr>
<td>Propane</td>
<td>0.65</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>0.59</td>
</tr>
<tr>
<td>Pentane</td>
<td>0.10</td>
</tr>
<tr>
<td>Butane</td>
<td>0.016</td>
</tr>
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The typical composition of NG is given in Table 2.1. The main constituent of NG is Methane, with chemical formula of CH$_4$ which has a relatively low C to H rate compared to fossil fuels as shown in Table 2.2, hence NG is considered to be a relatively clean fuel, less prone to soot formation during combustion than diesel, and with lower CO$_2$ emission potential. Though NG itself is not a renewable energy, its main constituent methane can be produced in a renewable way [29-31]. All of this makes NG a very attractive alternative fuel option for transportation. However, despite its advantages, NG
also has its own drawbacks as a fuel for vehicles. Its low energy density (CNG), difficulty of storage and transportation and lack of dedicated fueling infrastructures [32] are posing challenges that prevented it from being widely used in the past.

Table 2.2. Chemical formula and physical property of methane, gasoline and diesel [33]

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Methane</th>
<th>Gasoline</th>
<th>Light diesel</th>
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<tr>
<td>Chemical Formula</td>
<td>CH₄</td>
<td>CₙH₁.₈₇ₙ</td>
<td>CₙH₁.₈₇ₙ</td>
</tr>
<tr>
<td>Lower Heating Value (MJ/kg)</td>
<td>50.0</td>
<td>44.0</td>
<td>42.5</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>0.72</td>
<td>750</td>
<td>850</td>
</tr>
<tr>
<td>Octane Rating (RON)</td>
<td>120</td>
<td>92-98</td>
<td>-</td>
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</tbody>
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Nevertheless, NG has shown success in its usage in transportation in many countries. In the worldwide Light Duty (LD) vehicle market, Middle East countries and South American countries are demonstrating high market share in Natural Gas Vehicles (NGV). Iran, Pakistan and Argentina are the top 3 countries in terms of LD NGV vehicle populations, where NGV consists 80% of total LD vehicles in Pakistan. In the medium duty (MD) and HD vehicle market, China and Ukraine holds the largest number of NG fueled buses and trucks. Where in Ukraine, 72% of HD trucks are powered by NG. In contrast, US has the largest vehicle population in the world, its NGV market share is less than 0.1% in both LD and HD sectors [34].

To boost usage of NG in current road transportation vehicles, current engines require conversion to NG or dual-fuel operation. The conversion from existing HD CI engines to NG-fueled engines incurs additional cost, which to some extent counterbalances its fuel economy benefits. Thus, converting engines with high mileage
traveled per year will be the favorable option. The annual amounts of fuel used by HD trucks are 21\% of total fuel used by the transportation sector in 2013. The projection of this number to 2040 is 28\%. [35]. Given the Vehicle Miles Traveled, conversion of HD diesel to NG or dual-fuel operation is the most rapid and effective way of increasing NG utilization for transportation [7].

**Existing Options to Use Natural Gas in HD Engines:**

**Spark Ignited Natural Gas Engines**

To utilize NG in HD engines, two major options are spark-ignited NG only and CI dual-fuel engines. Most NG Engines currently offered by OEMs are conversions to SI combustion. The compression ratio is lowered compared to diesel to avoid knock. As shown in Table 2.2, even though methane has much higher octane rating than that of gasoline, the compression ratio has to be lowered to less than 13:1; additionally, the engine operates with stoichiometric mixture to enable application of a TWC for cleaning up the exhaust, hence the high efficiency traits associated with diesel engines including high compression ratio and lean operation are compromised.

Recent development of lean burn NG SI engines shows potentials of improving NG engine efficiencies. Unlike gasoline, NG engines can run a leaner mixture without compromising combustion stability [36]. The lean mixture yields a higher thermal efficiency compared to that of stoichiometric NG engines due to improvement of heat capacity ratio $\gamma$. Another benefit of lean burn NG engines comes from reduced pumping loss. At many load conditions, the throttle can operate at wide open position while load
control is realized from varying A/F ratio. However, lean burn NG engines induce challenges in exhaust treatment since conventional TWCs only work with stoichiometric mixture. To curb the NOx emissions, lean burn engines generally run close to lean limit to minimize combustion temperature. However, an oxidation catalyst will be required to clean up CO and HC emissions [37-41]. Another potential issue of running NG engine close to lean limit is combustion instability. Due to the low flame propagation speed of methane [33] and lean NG-air mixture, combustion duration becomes excessively long, which poses difficulties to combustion phasing control and penalizes thermal efficiency. At high load conditions, the slow NG flame propagation speed will increase the likelihood of knock. Recent studies found that with an addition of high reactivity fuel, i.e. hydrogen, the lean limit of NG-air mixture can be improved, as well as cycle-to-cycle variations. With the presence of hydrogen, flame propagation speed is improved, and results in faster combustion and improved thermal efficiency [42-51].

In summary, NG fueled SI engines display several drawbacks, namely 1) Low VE: Most of SI NG engines use port fuel injection, where air and fuel mix in the intake manifold. According to Table 2.2, methane has a much lower density than that of gasoline, thus part of the intake charge will be displaced by NG, resulting in lower volumetric efficiency. 2) Reduced compression ratio to prevent knock. 3) Difficulties in designing an effective NOx catalyst for lean SI NG operation, which force utilization of a three-way-catalyst (TWC) and stoichiometric operation. 4) Use of throttle, which induces pumping losses. All these facts hinder SI NG engines from competing with diesel engines in terms of efficiency. Furthermore, their deployment depends entirely on the availability
for re-fueling infrastructure in a given geographical region, thus the drivers’ range anxiety become a significant challenge.

Dual-fuel Engines

Dual-fuel NG-diesel engines offer an interesting alternative. In the case of a dual-fuel engine, the conversion from a conventional diesel engine requires little modification of engine hardware. High compression ratio is retained, and the engine can operate lean; hence, there is a prospect of achieving roughly the same thermal efficiency as in the case of a diesel baseline. Most dual-fuel engines are designed to work interchangeably in diesel-only or dual-fuel mode. This eliminates driver range anxiety, since the vehicle can continue running on diesel fuel if a NG filling station is not available.

The common configuration of a dual-fuel engine has a NG injector located in the intake upstream of the manifold. The NG mixes with fresh air and EGR in the intake system and is then inducted into the cylinder during the intake stroke, where mixing continues due to charge motion. As piston moves towards the end of compression stroke, a “pilot” spray of diesel is injected into the cylinder. After a short ignition delay period, the NG and air mixture is then ignited via the energy released by the combustion of the diesel spray. While in SI engines, the slow flame propagation speed contributes to cycle to cycle variations and lowered thermal efficiency, in dual-fuel engines this tends to be less a problem. In SI NG engines NG-air mixture is ignited by single ignition source which is spark plug. By contrast, dual-fuel engines generate multiple ignition points from the combustion of diesel spray. Previous research has demonstrated that even a very
small quantity of diesel spray generates much more ignition energy than that of a spark plug [52]. In typical SI NG engines NG flame has to propagate from a single ignition site through the entire charge, while in dual-fuel engines multiple flame front propagate simultaneously, results in a faster combustion and lowered lean limit [32]. In the light of this, dual-fuel engines can run un-throttled, which is another great advantage over SI NG engines.

**Review of Dual-fuel Engine Research**

Early research effort on dual-fuel NG diesel engines was pursued by Karim et.al [5-7, 9, 53]. Some issues including knock and combustion instability were observed and investigated in detail. At higher load conditions, a combination of the flame propagation through the NG-air mixture and a high compression ratio brings a risk of knock. Given the large bore diameter and low reciprocating speed of heavy duty engines, knock becomes a limit of dual-fuel engines, especially at high loads where NG substitution rates are elevated. On the other hand, at low load conditions, dual-fuel engines are subjected to combustion instability due to slow flame propagation in an overly lean mixture. The use of higher amount of pilot or hot residual gas can help alleviate this tendency [6]. Heat release characteristics of dual-fuel engines were also discussed in this study. It was observed that heat release of dual-fuel engines can be separated into two distinct phases, with first stage being contributed by the combustion of diesel pilot and part of gaseous fuel and second stage being much slower, driven by the combustion of remaining gaseous fuel.
The performance and emission characteristics of dual-fuel engines has been extensively studied. Generally the compression of diesel engine can be retained while dual-fuel mode generates power level close to diesel baseline. Some published work pointed out that the compression ratio should be limited to no more than 16.5 to achieve knock-free operation [54]. The same study also gives a comprehensive comparison between diesel baseline and dual-fuel engines in terms of engine performance. The efficiency of dual-fuel engine is somewhat lower than diesel baseline at low load but showing a close match with diesel baseline at moderate to high load. The reduced fuel conversion efficiency at low load is due to the poor flame propagation through the lean NG-air mixture, leading to incomplete combustion. In that case, the unburned NG exists in the exhaust. At higher load, where NG-air mixture is richer, dual-fuel combustion is exhibiting thermal efficiency close to a diesel baseline. A longer ignition delay period is observed with dual-fuel operation, which is also documented in several other studies [12, 55]. This is due to reduced diesel quantity injected, a prolonged chemical delay caused by the presence of gaseous fuel in the fresh charge and a reduction of charge temperature due to the high specific heat capacity ratio of NG [55].

Performance of Dual-fuel Engines

Krishnan et al.[12] investigated the effect of NG substitution rate on combustion characteristics of dual-fuel engines. Here, the NG substitution rate is defined as the percentage of NG energy relative to total fuel energy. It was observed that higher NG substitution rates have negative effect on combustion efficiency due to prolonged
combustion duration. On the other hand, high NG substitution rates result in delayed peak cylinder pressure, which lowers the combustion noise compared to diesel baseline. A longer ignition period and higher coefficient of variation (COV) of cylinder pressure is also observed with increase of NG substitution rate. The high COV at high NG substitution rate conditions is a major concern of the application of dual-fuel engines. The effect of intake temperature on dual-fuel combustion is also investigated. An improvement of fuel conversion efficiency was observed with higher intake temperature, due to improved NG flame propagation speed in a hotter NG air mixture. Additionally, hot intake gas results in a higher mass fraction burned of NG, which improves combustion efficiency and mitigates the methane slip problem. However, hotter intake gas increases the likelihood of knock. The prevention of knock acts as a limit for the charge temperature. Another important factor on combustion efficiency of dual-fuel engine is the equivalence ratio. Here the equivalence ratio is referring to the total equivalence ratio where both diesel and NG are considered. It is observed that fuel conversion efficiency increases with higher total equivalence ratio. Note that at high equivalence ratio cases ($\phi > 0.5$), fuel conversion efficiency of dual-fuel combustion exceeds the diesel baseline, as shown in Figure 2.3. Similar trend is also observed with increase of engine load, which is mostly depended on total equivalence ratio. While in reference [54], dual-fuel thermal efficiency was shown to be lower than that of diesel baseline, a reduced compression ratio was used in the dual-fuel engine, which accounts for part of the efficiency loss. Papagiannakis et al. observed similar trend as shown in Figure 2.3 in an independent study, where dual-fuel combustion exhibited higher brake
specific fuel consumption (BSFC) than diesel baseline at low load, while at high load, dual-fuel combustion was shown to have BSFC similar to diesel baseline. In that study, BSFC was obtained by measured engine-out power and fuel flow rate, thus the difference of lower heating value (LHV) between NG and diesel was not considered. Since NG has a higher LHV than diesel, the BSFC number of dual-fuel combustion would be higher if the difference of LHV between these two fuels were corrected [14]. It can be concluded that at same engine configurations, dual-fuel engines have potential of achieving similar level of efficiency as diesel engines.

![Figure 2.3. Fuel conversion efficiency and BSEC as function of total equivalence ratio.][12]

**Emissions of Dual-Fuel Engines**

Dual-fuel engines are known for producing less NOx and soot emissions than diesel engines [13, 14, 54-65]. The reduction of NOx emissions is mainly due to the
lowered combustion temperature and reduced oxygen concentration in the combustion chamber [14]. As mentioned in the above discussions, dual-fuel combustion yields lower peak combustion temperature compared to diesel engines under same speed and load due to prolonged combustion duration. The presence of gaseous fuel in the combustion chamber reduces oxygen concentration since part of air charge is replaced by gaseous fuel. Figure 2.4 gives a comparison of NOx emissions from diesel and dual-fuel engines under various load and speed conditions. It is shown that dual-fuel combustion yields less NOx emissions than diesel only under the same speed and load points. At low load and high speed conditions, the difference is not significant while at high load conditions, dual-fuel combustion produces considerable lower level of NOx than diesel only.
Karim et al. [66] suggested that NOx emissions of dual-fuel engines are strongly associated with the pilot diesel fuel. In dual-fuel combustion, burning of pilot diesel fuel results in high local temperature zones which are favorable for formation of NOx, while when combustion progress to premixed burning of NG, local combustion temperature is considerably lower. An increasing trend of NOx was observed with larger quantity of pilot fuel. Additionally, similar to the trend shown in Figure 2.4, lower NOx level was observed with smaller total equivalence ratio. It can be concluded that lower utilization of pilot fuel, together with low overall equivalence ratio is most beneficial for curbing NOx emissions in dual-fuel engines.

Dual-fuel engines generally produce much less soot emissions than diesel engines, in some cases the soot level is un-detectable [14, 55, 67, 68]. Figure 2.5 gives a comparison of soot emissions from diesel and dual-fuel engines under various load and speed conditions. The low-soot property of dual-fuel combustion is attributed to multiple factors. First of all, the main constituent of NG is methane, which is a fuel without carbon-to-carbon bonds. The carbon-to-carbon bond is a substantial factor for soot formation. Fuels with more carbon-to-carbon bond tend to generate more soot during combustion [32, 69], thus NG is an intrinsically low-soot fuel compare to diesel. Additionally, in most dual-fuel engines NG is introduced upstream of the intake, thus NG has sufficient time to mix with air prior to combustion. This eliminates locally rich fuel-air zones which otherwise creates favorable conditions for soot formation. The soot
emission of dual-fuel combustion are formed during pilot diesel fuel burning stage. Since NG continues to burn after the consumption of pilot fuel, it further oxidize the soot particles generated from pilot combustion. All these factors contribute to the low-soot characteristics of dual-fuel combustion.

Figure 2.5 Comparison of soot emissions under diesel only and dual-fuel operation at various load and speed conditions [14].

Although dual-fuel engines have significant advantage in terms of NOx and soot emissions over conventional diesel engines, they tend to produce more CO and HC emissions, especially at low load conditions [14, 55, 66, 67, 70-72]. CO and HC emissions of dual-fuel engines are mainly resulted from incomplete combustion of NG.
Since dual-fuel engines run un-throttled, low load conditions are associated with a low overall equivalence ratio, which is not a favorable condition for the flame propagation of NG. At extremely low load conditions, NG ignited by pilot spray may fail to propagate through the entire chamber. Additionally, due to the low laminar flame speed of NG, combustion extends late expansion cycle, when bulk gas temperature drops, and bulk quenching may occur before the flame reaches the walls. In that case, unburned NG and CO escape into exhaust. Krishnan et al. reported a NG combustion efficiency less than 80% in a test case when the engine operated at ¼ load. Other contributing factor of unburned fuel in the exhaust are wall quenching and NG trapped in the crevice volume [32]. Figure 6 gives a comparison of CO and HC emissions under diesel only and dual-fuel operation at various load and speed conditions. It is clearly shown that dual-fuel combustion produces significantly higher CO and HC emissions compared to diesel only, especially at low load conditions. As engine load increases, a significant reduction of CO and HC is observed. This is due to improved NG flame propagation and elevated combustion temperature which is favorable for oxidizing CO and HC [64].
Figure 2.6 Comparison of CO and HC emissions under diesel only and dual-fuel operation at various load and speed conditions (from [14]).

The phenomenon of unburned NG escaping with exhaust is also referred to as methane slip. This phenomenon rises environmental concerns since NG has greenhouse effect as much as 34 times of CO2 [73]. Several approaches have been developed to reduce the quantity of unburned NG. Karim et al. proposed increasing pilot fuel quantity to improve combustion efficiency at low load since a large amount of pilot fuel provides a stronger ignition source. Approaches based on reducing excess air were also proposed, including throttling the intake air and skip firing, where some of cylinders work in diesel only while rest of cylinders operate in dual-fuel mode with a higher equivalence ratio [66]. Other approaches such as intake gas heating, increase water jacket temperature, addition of high reactivity fuel (hydrogen) and use of hot EGR are also proposed to enhance the flame propagation through the lean NG-air mixture [65-67].
Direct Injection of NG in Dual-fuel Engines

Most of dual-fuel engines use fumigation, in other words, intake port fuel injection of NG. Due to its gaseous state, NG displaces a considerable amount of air in the cylinder charge, and this results in a lowered VE. To address this, some publications have demonstrated success in using direct injection of NG in dual-fuel engines [62, 74-78]. In these articles dual-fuel engine with DI of NG are referred as High-Pressure Direct Injection (HPDI). HPDI dual-fuel engines are reported to produce similar level of power and thermal efficiency compared to diesel baseline. Under some test conditions, thermal efficiency improvement of 5% and engine load capacity improvement of 20% compared to diesel baseline were reported [62]. In a HPDI dual-fuel engine, a unit-type injector capable of injecting both diesel and NG substitutes the original diesel injector. As piston moves towards the end of compression stroke, the injector first injects a small quantity of diesel pilot spray, followed by direct injection of NG. The injection pressure of NG was reported as 100-160 bar in the early development stage [62] while in later published work the injection pressure was reported to increase up to 200-300 bar [78]. Since NG is injected late in the compression stroke, the engine is no longer knock-limited, this allows engine to run at high compression ratio, resulting a high engine specific power output [62]. HPDI dual-fuel engines are also documented to produce lower level of NOx and soot emissions compared to baseline diesel combustion. However, a direct comparison on NOx and soot emissions between port fuel injected and HPDI dual-fuel engine was not reported. Method of NOx reduction in HPDI engines are retarded timing of pilot diesel
injection [62] and dilution of intake charge [78]. Retard of pilot injection reduces NOx emission but meanwhile it has negative effect on soot emissions and engine thermal efficiency. A desirable compromise needs to be determined to lower the NOx emissions while maintain desirable thermal efficiency. The effect of NG injection pressure on engine performance and emissions was also studied [78]. A higher NG injection pressure results in a shortened ignition delay, due to fast mixing of pilot fuel and surrounding air. However, this had negative effect on NOx emissions due to faster heat release rate and elevated combustion temperature. Figure 2.7 shows the effect of NG injection pressure on engine out emissions under conditions with or without intake charge dilution. It is shown that under condition without EGR, NOx emissions increase with increase of NG injection pressure while soot emissions show reverse trend. With addition of EGR, NOx emission is dramatically reduced and is not greatly affected by varied injection pressure. High injection pressure combined with intake dilution displays simultaneous reduction of HC and soot, while NOx remains at a much lower level compared to the case without EGR. It is concluded that HPDI is a promising technique for utilizing NG in heavy duty engines due to its potential of achieving similar or higher engine output, together with knock-free operation and high thermal efficiency. However, this concept is subjected to high installation cost since the original diesel injection needs to be replaced, cylinder head requires a modification, and the injector (diesel + NG) is much more expensive and not as reliable as a standard. Also, range anxiety remains an issue in HD truck applications.
Advanced Diesel Injection in Dual-Fuel Engines

In the last decade of dual-fuel research, increasing NG substitution rate, i.e. reduction of the fuel quantity in the pilot injection has been one of the key research objectives. The benefits of using a small pilot and potential complication has been documented in literature [52, 57, 60]. In recent years, an Advanced Low Pilot Ignited Natural Gas engine (ALPING) concept was proposed [15-18, 71]. This concept features a very advanced (up to 60 BTDC), small amount of diesel pilot as the ignition source, with the port fuel injected NG as the main heat release source. In this case, diesel fuel only provides energy for ignition while load control is realized by varying the quantity of NG. ALPING engine is a marriage of pilot-ignited dual-fuel engines and homogeneous charge compression ignition (HCCI) engines. Due to advanced pilot injection, the onset of combustion is predominately controlled by chemical reactions. While HCCI engines suffer from combustion control challenges at high or low load, the high Cetane fuel
(diesel) in ALPING engines acts as stable ignition source for the NG-air charge. The major benefit of the ALPING concept is the reduction of NOx emissions. In conventional dual-fuel engines, reduction of NOx is generally achieved by retarding pilot injection timing, but this penalizes fuel conversion efficiency and engine performance [61]. In comparison, ALPING use advanced diesel pilot injection (45~60 deg BTDC), results in a long ignition delay and better charge mixing. The better mixing of diesel and surrounding air and natural gas mixture also helps the ignition of NG, resulting in lower local temperatures and reduced NOx emissions. Meanwhile, better diesel fuel and air mixing reduces the rich pockets of diesel fuel and minimizes soot emissions [71].

Figure 2.8 Effect of pilot injection timing on NOx emissions and fuel conversion efficiency (from [71])

Figure 2.8 shows the effect of pilot injection timing on engine out NOx emissions and fuel conversion efficiency at part load and full load conditions. It is shown that advanced pilot injection timing (before 40 BTDC) has a significant effect on reduction of NOx while high fuel conversion efficiency is maintained. However, ALPING engine is subject to combustion instability issues. Incomplete combustion occurs at low load due to
the low temperature combustion nature of the cycle[71]. The bulk quenching of flame due to poor flame propagation under low temperature and lean mixture conditions, as well as flame quench near the wall cause more unburned HC emissions, or methane slip, compared to conventional dual-fuel engines. Suggestions for improving low load combustion stability and HC emissions include higher intake temperature and higher quantity of pilot fuel [15]. However, both methods result in a penalty on NOx emissions.

**Modeling of Dual-fuel Combustion**

Extensive modeling work of dual-fuel combustion has been conducted in published work. These combustion modeling approaches are classified into 3 categories:

1. 0-D Model

   0-D models include semi-empirical model such as Wiebe model [4, 6, 10, 64, 79-83]. Wiebe models have no spatial resolution and are generally used for heat release analysis. The heat release analysis from measured cylinder pressure information has been applied to dual-fuel engines for characterization of combustion modes [66, 84-86]. The introduction of gaseous fuel into combustion chamber greatly alters the combustion characteristics of conventional diesel engines. A dual-fuel engine involves features from both CI and SI engines. The fuel injection process includes in-cylinder direct injection of diesel and port fuel injection of NG. The ignition process includes auto ignition of diesel, multi-site ignition of NG ignited by adjacent diesel flamelets, which is followed by both premixed and diffusion combustion of diesel and flame propagation of NG. Since two types of combustion occur simultaneously in a shared space, it is difficult to analyze the
combustion process from simply examining the total heat release profile. Previous literature [10, 66, 87] has established models that separate the heat release contributions of each fuel. However, these models are mainly applicable to dual-fuel engines where only a small quantity of diesel to serve solely to ignite NG. As the amount of diesel fuel injected varies, the interaction of NG-air mixture with diesel spray and ignition characteristics are altered correspondingly. Due to their semi-empirical nature, 0-D combustion models are not predictive and require extensive calibration. However, they contain enough physics for accurate calculations of gas flow through the valves, compression and heat transfer. Modeling of manifolds as separate control volumes allows integration of individual cylinders, a turbocharger, and various elements in the intake and exhaust to create a complete engine system.

2. Quasi-D Model

Quasi-D modeling of the dual-fuel combustion provides a good compromise between predictive capabilities and computational efficiency [17, 18, 70, 87-92]. Papagiannakis et al. proposed a phenomenological multi-zone flame propagation model of NG combustion under dual-fuel environment [70]. The flame front of NG combustion was assumed as a conical shape surrounding the diesel spray and propagates through the unburned NG-air zone over time. The interaction between NG flame front and wall was also considered. As shown in Figure 2.9, geometrical definition of flame front before and after wall impingement is given. The burn rate of NG is obtained by calculating rate of change of burning zone volume. In this phenomenological dual-fuel combustion model,
flame overlap between each “cone” is not considered. The heat release contribution of diesel fuel is estimated by a 0-D Arrhenius type reaction rates correlation.

Figure 2.9 Illustration of burning zone. Left: before wall impingement, Right: After wall impingement (from [70])

Krishnan et al. proposed a multi-zone model for ALPING combustion [18]. The model applied diesel spray-combustion model and a NG turbulent flame propagation model. The cylinder volume was divided into 4 zones: an unburned zone, a pilot fuel zone which accounts for diesel combustion, a NG flame zone for combustion of NG and a burned zone with products of combustion. Figure 2.10 gives an illustration of zone separation in this modeling approach. Diesel combustion is addressed using a packet model, while the burn rate of NG was calculated from a turbulent flame propagation model, where the flame front area is defined as:

$$A_f = K_{AF} \sum_{n=1}^{n_{zon}} y_{p}^{C_A} V^2/p^{2/3}$$

(2.1)
where \( A_f \) is the flame front area, \( K_{AF} \) and \( C_b \) are model parameters, \( n_{\text{preset}} \) is the number of ignited packets, \( y_{pb} \) is packet burned mass fraction and \( V_p \) is the packet volume. The limitation of this modeling approach is: 1). the flame of NG was assumed to initiate from each diesel packet and for simplicity reason, no interaction, overlapping or combined enflamed areas are considered between packets. 2). This model was proposed for partially premixed ALPING low temperature combustion (LTC). The diesel spray in this case only accounts for a very small amount of energy content (2%-3%). Also, because of early injection (>40 deg BTDC), diesel spray is well premixed with air before combustion. Thus the combustion characteristics are very different than dual-fuel engines running with conventional diesel injection timings and relatively lower NG substitution rates.

![Figure 2.10 Schematic diagram of zone evolution (from [18])](image)

3. 3-D Model
Detailed CFD models have the highest predictiveness and spatial resolution [17-24]. Generally, a 3-D simulation provides detailed spatial resolution of the combustion process and has high prediction accuracy. Previous 3-D simulation work has been conducted on dual-fuel concepts and it produced the insights about in-cylinder processes. However, the 3-D simulation comes with high computing cost, and it is not suitable for system level analysis or potential real-time applications. Rather, it is primarily intended for optimizing combustion chamber shape, and exploratory studies of advanced concepts.

4. Discussion and research direction

The three numerical modeling categories discussed above are widely used in engine related research, but each has a particular role. A 0-D model is ideal for system level study and applications where fast model execution is critical. However, the predictiveness and fidelity of this approach is highly limited. Due to its lack of spatial resolution, the spray and combustion characters of diesel fuel, as well as the flame propagation of NG cannot be represented from the model. Rather, prior knowledge from experiments is needed to tune the semi-empirical combustion model. On the other end of the spectrum, 3-D modeling approach is perfect for detailed characterization of combustion and CFD codes yield unprecedented spatial resolutions. Unfortunately, the computation requirements that comes with meshing the in-cylinder space and solving the governing equation in each cell are very high. Significant advancement of computer computing power is still needed before the 3-D CFD simulation can become viable for engine system studies.
This work aims to achieve an optimal compromise by developing a model with spatial resolution and fidelity that enable prediction of the in-cylinder combustion process while requiring moderate computation power. Execution speed should be sufficient for engine system studies, i.e. investigation of turbocharger matching, development of EGR strategies as well as fuel injection calibration. Real-time applications for control can easily be within reach too. Based on this, quasi-D modeling approach is the right choice for modeling the combustion process. The modeling of gas exchange process on the other hand, requires no spatial resolution, thus 0-D modeling is optimal due to its intrinsically low computation requirements.
CHAPTER THREE

ZERO-D ANALYSIS OF DUAL-FUEL COMBUSTION

Introduction

A predictive simulation of a complete turbocharged dual-fuel engine system is invaluable for characterization of injection strategies, transients, and development of strategies for improving the dynamic response. However, insights from experimental investigations are needed to establish a foundation for development of predictive models, and guide decisions about the most appropriate approach. Heat release analysis has been routinely applied to diesel engines for characterization of combustion modes. [66, 84-86] The introduction of gaseous fuel into combustion chamber greatly alters the combustion characteristics of conventional diesel engines. A dual-fuel engine involves features from both compression ignition and spark ignition engines. [87] The fuel injection process includes in-cylinder direct injection of diesel and port fuel injection of NG. The ignition process includes auto ignition of diesel, multi-site ignition of NG by adjacent diesel flamelets, which is followed by both premixed and diffusion combustion of diesel and flame propagation of NG. Since two types of combustion happen simultaneously in a shared space, it is difficult to analyze the combustion process from simply examining the total heat release profile.

Previous published work [10, 66, 87] has established models that separate the heat release contributions of each fuel. However, these models are mainly applicable to dual-fuel engines where only a small quantity of diesel to serve solely to ignite NG. Instead,
this study investigates NG substitution rates as low as 30% by energy content, thus, and in this case diesel fuel plays a more substantial role than just an ignition source. As the amount of diesel fuel injected varies, the interaction of NG-air mixture with diesel spray and ignition characteristics are altered correspondingly.

The objective of the work in this Chapter is to develop a combustion analysis tool to investigate: (i) ignition delay of diesel fuel, and (ii) heat release contribution from the gaseous NG during dual-fuel combustion over a range of NG substitution rates. The approach is based on a Zero-D heat release model derived from cylinder pressure data. A Zero-D model requires little computing effort, and the idea is to extract sufficient information from experiments and develop a semi-empirical combustion model capable of creating a predictive-enough tool for engine system studies. In this study, in-cylinder pressure measurements were obtained on a 15 liter HD Diesel engine modified for dual-fuel operation. Insights from this study will be utilized to guide the subsequent effort on developing a predictive, Quasi-D dual-fuel combustion model.

The approach relies on a Triple-Wiebe function as heat release analysis model. Triple-Wiebe model is first calibrated using baseline diesel combustion data. Injection timing and start of combustion are derived from experiments. An equivalence ratio based ignition delay correlation is validated with diesel only combustion. The premixed fraction of diesel only combustion is investigated by relating the heat release shape to the distribution between premixed burn and mixing controlled burn. Subsequently, a similar concept is applied to dual-fuel operation. The ignition delay period of dual-fuel combustion is estimated with a predictive correlation, and the effect of equivalence ratio
on the successful prediction of ignition delay is also examined. A pseudo equivalence ratio is defined in order to improve predictiveness.

A four stage heat release mechanism for dual-fuel operation is proposed, where NG heat release is composed of multi-site ignition and flame propagation. To determine the relative fractions of NG ignited by diesel flame and consumed by flame propagation, the heat release distribution of each stage is analyzed with a Triple-Wiebe function. The influence of NG equivalence ratio and substitution rate on multi-site ignition fraction is also examined.

Transient analysis of a dual-fuel engine system carried out here is motivated by experimentally observed drivability issues. In real world operation, during tip-in or tip-out conditions, drivers have experienced a lag in the dual-fuel engine response. Thus, a 1-D simulation tool is developed in GT-Power environment and applied to generate the required insight, and subsequently devise control strategies for smooth torque delivery under very dynamic conditions.

The baseline 1-D simulation represents the Cummins ISX HD engine. Data pertaining to intake and exhaust geometry, cam profiles and turbomachinery maps are used to configure the engine system. Variable geometry turbocharger (VGT) behavior is validated through experimental results. The triple Wiebe combustion model was calibrated based on experimental combustion results for both diesel and dual-fuel combustion. The ignition delay and injection timing are determined through an iterative calculation based on SOC and a predictive ignition delay correlation.
After a thorough validation of the simulation, the tool is utilized to investigate experimentally observed power delivery delays experienced during transient tip-in/tip-out conditions. A simulation of the transient event quantified the transport delay. This enabled development of the algorithm that manipulates the diesel injection quantity to compensate for the NG induction/transport delay. Finally, the algorithm is validated throughout the operating range.

**Experimental Apparatus**

Experimental investigation has been conducted on a chassis dynamometer with a Cummins ISX 550 dual-fuel engine mounted in the Class 8 HD truck. The baseline engine was calibrated to meet US EPA 2007 emission regulation, and modified to operate with a NG fumigation system. The engine is a turbocharged inline six, intercooled, with direct injection. Diesel fuel pressure is generated from an injector plunger pushed by an injector rocker, actuated by the fuel cam. The injection timing and quantity are controlled by varying the volume of fluid within the two injector chambers. NG injector is installed upstream of intake manifold after the compressor, where NG and air are mixed. To accommodate the required NG flow, three Clean Air Power NGV solenoids with 125 psi injection pressure were mounted in a custom designed manifold 120 degree apart around the circumference. The solenoids were fired in a sequence, with significant overlap between injectors adjacent in the firing order. This arrangement allowed each solenoid some dwell time while closed to avoid overheating.
Table 3.1. Engine specifications

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Diesel/Dual-fuel 4-stroke</th>
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<tbody>
<tr>
<td>Configuration</td>
<td>In-line 6-cylinder</td>
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<td>Air intake</td>
<td>Turbocharged, intercooled</td>
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<tr>
<td>Fuel type</td>
<td>Diesel D2, Natural gas</td>
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<tr>
<td>Diesel Injector type</td>
<td>Unit injector</td>
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<tr>
<td>Firing order</td>
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<td>Displacement</td>
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<td>Bore</td>
<td>137mm</td>
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<tr>
<td>Stroke</td>
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<tr>
<td>Connecting rod length</td>
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<tr>
<td>Compression ratio</td>
<td>17:1</td>
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<td>Rated power/rpm</td>
<td>405kW@2000rpm</td>
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Table 3.2. Composition of natural gas used in the experiment.

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole fraction (%)</th>
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<tbody>
<tr>
<td>Methane</td>
<td>95.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>3.2</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0.5</td>
</tr>
<tr>
<td>Propane</td>
<td>0.2</td>
</tr>
<tr>
<td>iso - Butane</td>
<td>0.03</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0.02</td>
</tr>
<tr>
<td>iso - Pentane</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Figure 3.1: Experimental instrumentation on the Cummins ISX dual-fuel engine

The cylinder head was modified to install knock resistant GH15DK piezoelectric pressure transducers in cylinders 5 and 6. Cylinder pressure signals were amplified by MICROIFEM piezoelectric amplifiers within an AVL IndiSmart data acquisition. National Instruments CompactDAQ with 9205 and 9213 series modules was utilized to sample additional signals. Diesel fuel flow was measured by an AVL KMA Mobile; NG and air flows were measured using FOX FT2 inline flowmeters. Turbo shaft speed was measured by a PicoTurn rotational speed sensor. Air temperature, oxygen sensors, manifold pressure and other additional sensors were mounted on the engine for comprehensive data acquisition. Voltages sent to the two injection solenoids from the ECU were tapped and sent through the crank angle resolved data acquisition system to quantify both the fuel quantity in the injection chamber and the fuel quantity sent to the timing chamber. The complete list of measured signals is as follows:

**Time based:**
- Intake manifold air pressure
- Exhaust manifold air pressure
- Intake gas temperature
- Exhaust gas temperature
- Intake equivalence ratio
- Exhaust equivalence ratio
- Turbo shaft speed
- Compressor inlet and outlet air pressure and temperature
- Turbine inlet and outlet air temperature and pressure
- Diesel, NG and air flow rates
  
  **Crank angle based:**

  - Cylinder pressures
  - Engine knock

The truck was tested on a chassis dynamometer, and engine speed-load sweeps were carried out for both diesel-only and dual-fuel operation. Figure 3.2 illustrates cyclic and cylinder to cylinder variations of measured cylinder pressure data from a dual fuel operation case. Coefficient of variation (COV) of indicated mean effective pressure (IMEP) in cylinder 5 and cylinder 6 are 1.4% and 1.2%, respectively. Ensemble averaged cylinder pressure information from 500 consecutive cycles was used for heat release analysis and the comprehensive data set listed above enabled validation of both in-cylinder process and turbocharged engine system behavior. Due to the complexity of the unit-injector design, installing a Hall Effect sensor for measuring needle lift was not an
option; therefore, an approach based on the heat release analysis was devised to infer start-of-injection from cylinder pressure data.

Figure 3.2: Cyclic and cylinder to cylinder variations of measured cylinder pressure data

**GT-Power Engine Modeling**

A comprehensive 1-D simulation of the Cummins ISX 550 dual-fuel NG diesel engine is developed in GT-Power. A schematic of the model is shown in Figure 3.3.
Figure 3.3: GT-Power model of the Cummins ISX dual-fuel engine

The intake and exhaust geometry have been carefully measured and used to configure the model. An accurate profile of the exhaust manifold is crucial for yielding satisfactory results because gas dynamics produce effects on both VGT and EGR. Figure 3.4 shows a layout of the exhaust manifold geometry on the Cummins ISX engine utilized in the simulation model.

Figure 3.4: Exhaust manifold geometry of the Cummins ISX engine
The intake and exhaust valve lift profiles were measured on the camshaft. Since the head was removed from the engine during profile measurement, instead of referencing the TDC to the crankshaft, an OEM wedge was applied to a slot on the camshaft and set as a reference point. The reference point was not necessarily the actual TDC position because a small free play exists between the wedge and the camshaft. Hence the TDC position was further calibrated in the GT-Power model for enhanced accuracy.

The turbocharger on the dual-fuel Cummins ISX engine is a Holset VGT™. In the simulation model, the turbocharger maps are scaled from existing examples of compressor and turbine maps to match experiment data at various operation points. VGT actuation positions are also inferred from the experiment data.

Figure 3.5 shows a comparison of simulated and experimental gas exchange process. In this case the engine operated in diesel mode at 1200 rpm at IMEP of 12 bar. The model accurately captured the intake and exhaust gas dynamics. Similar agreement was achieved at other speed/load points.
The NG injector is located between the outlet of the intercooler and the intake manifold. The experimentally measured NG mass flow rate is used to control the injection quantity in the simulation model. The diesel injectors used in the experimental engine are 9-hole unit-injectors with 0.186 mm nozzle holes and maximum injection pressure of 2200 bar. The injected mass and injection timing information are stored in 2-D look-up tables as a function of engine speed and IMEP. Likewise, injection pressure information is stored in 1-D look-up table as function of engine speed only.

Heat Release Analysis: Baseline Diesel Operation

A comprehensive heat release analysis is applied to diesel only operation as a baseline. In this section, a method to infer diesel injection timing from heat release profile is given. Experimental cylinder pressure data was analyzed to produce the heat release
profile as defined in Equation (3.1) [33], where $Q$ is energy released from the combustion of fuel, $\theta$ is crank angle, $\gamma$ is the specific heat ratio, $p$ is measured cylinder pressure, $V$ is the instant cylinder volume and $dQ_{ht}/d\theta$ is the convective heat transfer rate to the cylinder wall, which is defined in Equation (3.2). In the heat transfer calculation, $A$ is cylinder surface area, $T$ is mean gas temperature, $T_w$ is the mean wall temperature during compression, which is set as constant 400K. The $h_c$ is Woschni heat transfer coefficient [93], defined in Equation (3.3), where $B$ is the cylinder bore and $w$ is the cylinder gas characteristic, given in Equation (3.4), where $S_p$ is mean piston speed.

$$
\frac{dQ}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{dQ_{ht}}{d\theta} \tag{3.1}
$$

$$
\frac{dQ_{ht}}{dt} = Ah_c(T - T_w) \tag{3.2}
$$

$$
h_c = 3.26 B^{-0.2} p^{0.8} T^{-0.55} w^{0.8} \tag{3.3}
$$

$$
w = 2.28 S_p \tag{3.4}
$$

The cylinder gas temperature during compression process are calculated based on intake gas temperature, where isentropic compression neglecting heat transfer is assumed:

$$
T_{cyl} = T_{intake} \left( \frac{V_d}{V} \right)^{\gamma - 1} \tag{3.5}
$$

where $T_{intake}$ is intake gas temperature measured at intake manifold thus the effect of EGR gas is included, $V_d$ is cylinder displacement and $\gamma$ is the heat capacity ratio of in-cylinder charge. The inclusion of EGR alters the composition and thus the $\gamma$ of intake
gas. At room temperature, air has a $\gamma$ value of approximately 1.4 and EGR is slightly lower. In this work, EGR percentage used in the experiments ranges from 5% to 25%. An additional effect on $\gamma$ value is the temperature increase at the end of compression. We assign a constant value of 1.35 for $\gamma$ during the compression process to capture the combined effect of charge composition and temperature. Sensitivity of gas temperature estimation to $\gamma$ is studied and results are summarized in Table 3.3, where the differences of temperature estimation with varying $\gamma$ values compared to baseline ($\gamma = 1.35$) are given. Here the cylinder gas temperature at SOI is used for testing the sensitivity of temperature estimation. The ratio between cylinder displaced volume $V_d$ and cylinder volume at SOI $V_{SOI}$ ranges from 6 (advanced SOI) to 10 (late SOI) in the experimentally tested cases; this translates into a 30K temperature difference between an advanced and retarded SOI cases. It is shown that if the true $\gamma$ value falls into a 1.33 to 1.37 region, the estimation error of gas temperature at SOI is within 20K. The heat transfer term defined in Equation (3.1) is applied during compression process. This aids the determination of SOI by separating heat loss to the wall from heat absorbed by fuel evaporation. For combustion analysis, the heat transfer term is set to zero, and net apparent heat release rate is used for model calibration and validation.

Table 3.3 Sensitivity of gas temperature estimation to $\gamma$

<table>
<thead>
<tr>
<th>Intake Temperature [K]</th>
<th>$\frac{V_d}{V_{SOI}}$</th>
<th>Temperature estimation compared to baseline $\gamma = 1.35$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$T - T_{baseline}$ [K]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\gamma = 1.31$</td>
</tr>
<tr>
<td>310</td>
<td>6</td>
<td>-20.43</td>
</tr>
</tbody>
</table>
Start of diesel fuel injection can be inferred from heat release analysis. As diesel fuel is injected into the chamber, the fuel evaporation causes a dip in the heat release profile. The onset of this dip can be used as a criterion for SOI determination. However, heat release is a function of the first derivative of cylinder pressure, and signal fluctuations are magnified, thus hindering the accurate detection of heat release dip onset. Fourier transform is applied to filter the high frequency portion of heat release data and eliminate the noise, which is typically over $10^4$ Hz, while preserving the physical characteristics of the signal. The heat release is subsequently reconstructed with inverse Fourier function:

$$
\frac{dQ}{dt} = \frac{dQ}{dt_{\text{avg}}} + \sum_{n=1}^{N} [A_n \cos(n\omega t) + B_n \sin(n\omega t)]
$$

(3.6)

where $dQ/dt_{\text{avg}}$ is average heat release, $A_n$ and $B_n$ are Fourier coefficients, $\omega$ is angular frequency and $n$ is the harmonic number. Figure 1 shows the accuracy of Fourier reconstruction as a function of harmonic number. The Normalized Root Mean Square Error (RMSE) is calculated as:

$$
NRMSE = \sqrt{\frac{\sum (y-y')^2}{\bar{y}^2}}
$$

(3.7)

where $y$ is normalized heat release rate derived from measured cylinder pressure, $y'$ is normalized heat release rate from Fourier reconstruction or rolling average and $\bar{y}$ is
averaged normalized heat release rate. The selection criteria for harmonic number is to use smallest possible number able to insure minimal loss of accuracy. In Figure 3.6, RMSE of reconstruction reaches a steady minimum starting at $n = 12$ and this number remains unchanged over a range of engine operating conditions. Thus, a harmonic number of 12 is chosen. Figure 3.7 shows the effect of harmonic number on the reconstruction of heat release. The peak portion of the heat release profile is magnified. If the harmonic number is set too low ($n = 6$), the accuracy of reconstruction is lost. While a high harmonic number ($n = 25$) provides accurate reconstruction, it reintroduces undesirable fluctuations in the reconstructed heat release profile. For comparison, a rolling average of heat release is also shown in Figure 3.7. The Fourier reconstruction approximates the experiment data much more accurately than the rolling average, which displays an offset in both amplitude and phasing.

Figure 3.6 Normalized RMSE of heat release vs. harmonic number and comparison with rolling average method.
Figure 3.7. Comparison of Fourier reconstruction where various harmonic numbers were adopted

Figure 3.8 exhibits SOI determination via the Fourier heat release reconstruction during the initial stage of fuel injection and ignition. The reconstructed heat release profile accurately tracks experimental data and minimizes the disturbance from noise. The start of diesel fuel injection is determined via the intersection point of linear regressions fit prior to and after start of injection (SOI). SOC is selected at the minimum of the reconstructed heat release profile. This heat release rate (HRR) based SOI derivation method is only applied for diesel only conditions. For dual-fuel operation conditions, a method based on the information of injector pulse widths is used to determine SOI, which will be discussed in the later section of this work.
Diesel Fuel Injector Design and Injection Timing Prediction

In this section, a method to calculate SOI from experimentally measured diesel injection timing and metering solenoid pulse widths is given. A predictive ignition delay correlation for diesel only operation is then validated with experimentally derived ignition delay values.

Heat release based SOI determination suffers from several main drawbacks: (i) The heat release derived from experimental cylinder pressure is disturbed by noise, often requiring heavy filtering to minimize the noise interference, (ii) Qualitative determination of the inflection point is subjective, which introduces additional error, (iii) The inflection point corresponding to SOI can be difficult to select for some data points where lesser amount of diesel is injected. Figure 3.9 illustrates the challenges through an example of SOI determination for the case with lower amount of diesel fuel injected. The heat
absorbed by evaporation of fuel has a relatively weaker effect on the total heat release, adding difficulty to inflection point determination.

Figure 3.9. Another Example for Identification of SOI based on heat release analysis – it is difficult to detect the inflection point for a low load case.

More reliable SOI information can be obtained by combining heat release derived SOI data with examination of fuel injector geometry and recording of the solenoid pulse. The injection system in the tested engine is a unit-injector type. During a fuel injection event, as shown in Figure 3.10, the upper plunger is pushed downwards by the fuel cam to generate injection pressure. Injection quantity and timing are controlled by feeding fuel into the metering and timing chambers, respectively.
Start of injection is solely dependent on the plunger free travel, since fuel injection begins as soon as the lower plunger starts pushing the fuel in the metering chamber. Fuel quantity in timing and metering chambers is controlled by adjusting pulse widths of solenoid valves that feed fuel into these chambers, respectively. Since fuel pressure in the feed lines is regulated at 380 psi, the fuel quantity within the timing and metering chambers is a linear function of pulse width. The mathematical representation of the relationship between fuel quantity and pulse width is:
\[ V_{M,T} = \frac{c_1 \cdot \tau_{M,T} + c_2}{c_3} \]  

(3.8)

where \( V_{M,T} \) is fuel volume in the metering and timing chambers, \( \tau_{M,T} \) is experimentally measured metering and timing pulses and \( c_1, c_2, c_3 \) are constants calibrated with experiment data, which are same for both metering and timing chamber. Since the metering and timing chamber diameters \( d_M \) and \( d_T \) are constants in the vertical direction, the plunger free travel can be represented as a linear function of the fuel quantity in timing and metering chamber:

\[ h_{MF,TF} = h_{MT,TT} - \frac{4V_{M,T}}{\pi \cdot d_{M,T}^2} \]  

(3.9)

\[ h_F = h_{MF} + h_{TF} \]  

(3.10)

where \( h_F \) is plunger total free travel. \( h_{MT,TT} \) is maximum plunger travel in metering and timing chamber, respectively. \( h_{MF}, h_{TF} \) is lower and upper plunger free travel before it fully contacts with metering and timing fuel. With this correlation established, diesel SOI can be represented with a function solely dependent on the timing and quantity pulse widths.

Figure 3.11 shows total plunger free travel \( h_F \) calculated from injector solenoid pulse widths across the engine operating range in diesel-only mode. It is shown that plunger free travel is largely a function of engine load, or injected diesel quantity. However, this correlation is not sufficient to determine diesel injection timing on a crank angle basis without an accurate fuel cam profile.
At this point, SOI data acquired from diesel-only heat release analysis can be used to assess its relationship with timing and metering pulses. Figure 3.12 shows the SOI determined from heat release as a function of calculated plunger free travel over a load range. A linear regression is applied to correlate these two sets of data. The SOI function is now fully calibrated, and can be used in further studies to determine SOI directly from timing and metering pulses, i.e.:

\[
SOI = k_1 \sum_{i=M,T} h_i \left( \frac{4(c_1 \tau_i + c_2)}{c_3 \pi d_i^2} \right) + k_2
\]  

where \( i = M, T \) stands for metering and timing, respectively, \( k_1 \) and \( k_2 \) are constants calibrated with HRR derived SOI and calculated total free travel. The relevance is magnified in the context of this work, since Equation (3.11) can also be applied for dual-
fuel case, where HRR based SOI derivation is not an option due to reduced diesel injection amount and altered charge properties resulting in a less obvious HRR inflection. Due to the fact that the tested engine uses a unit-injector fuel injection system, the correlation given in Equation (3.11) is applicable only to engines equipped with such a systems. However, the heat release inferred method given in the previous chapter is applicable to any diesel engine.

![Figure 3.12. Linear regression fit of SOI derived from heat release analysis as a function of injector upper plunger free travel](image)

**Predicting Ignition Delay**

Prior to developing a predictive ignition delay model for dual-fuel combustion, a baseline ignition delay model is validated with diesel only combustion. In the present work, a predictive ignition delay correlation developed by Assanis et al. [94] is adopted:
\[ \tau_{ID} = 2.4 \phi^{-0.2} \bar{P}^{-1.02} \exp \left( \frac{E_a}{R_u \bar{T}} \right) \]  

(3.12)

where \( \phi \) is the global equivalence ratio, \( \bar{P} \) and \( \bar{T} \) are cylinder pressure and temperature at SOI, where temperature is calculated using Equation (3.5). As being discussed in the previous chapter, constant \( \gamma \) value of 1.35 is used for temperature estimation. The sensitivity of ignition delay prediction to \( \gamma \) due to the effect of EGR is summarized in Table 3.4. It is shown that if the true \( \gamma \) value falls into 1.33 to 1.37 region, the estimation error of ignition delay is within 8%. \( E_a \) is activation energy and \( R_u \) is universal gas constant. For diesel D2 fuel, Watson [85] suggested a value of 2100 for \( E_a / R_u \). Figure 3.13 illustrates accuracy of the ignition delay correlation applied to the baseline diesel only. Experimentally determined ignition delay values from the heat release analysis show a reasonable level of agreement with values calculated from Equation (3.12). Heat release data to derive SOI is from averaged cylinder pressure of 500 consecutive cycles at each steady state engine operating condition. To quantify the prediction accuracy, a correlation coefficient is calculated:

\[ SS_{res} = \sum_{i=1}^{N} (\tau_{exp, i} - \tau_{cal, i})^2 \]  

(3.13)

\[ SS_{tot} = \sum_{i=1}^{N} (\tau_{exp, i} - \bar{\tau}_{exp})^2 \]  

(3.14)

\[ R_{ID} = \sqrt{1 - \frac{SS_{res}}{SS_{tot}}} \]  

(3.15)

where \( \tau_{exp} \) and \( \tau_{cal} \) are experimentally observed and calculated ignition delay, respectively. \( N \) is the number of cases examined. The correlation coefficient \( R_{ID} \) between
the baseline ignition delay model and experimental data is 0.955. It is shown that experimental data is scattered evenly on both sides of calculated ignition delay, which indicates that there is no systematic error in either direction. The fluctuation of experiment data is caused by multiple factors: measurement noise, cyclic variations and SOI determination offset. The ignition delay correlation developed in this chapter is also used in the Quasi-D dual-fuel combustion model discussed in Chapter 5.

Table 3.4 Sensitivity of ignition delay prediction to $\gamma$.

<table>
<thead>
<tr>
<th>Intake Temperature [K]</th>
<th>$\frac{V_d}{V_{SOI}}$</th>
<th>Temperature estimation compared to baseline $\gamma = 1.35$ $(\tau_{ID} - \tau_{ID, baseline})/\tau_{ID, baseline} \times 100%$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\gamma = 1.31$</td>
</tr>
<tr>
<td>310</td>
<td>6</td>
<td>14.11</td>
</tr>
<tr>
<td>310</td>
<td>10</td>
<td>15.33</td>
</tr>
<tr>
<td>340</td>
<td>6</td>
<td>12.79</td>
</tr>
<tr>
<td>340</td>
<td>10</td>
<td>13.89</td>
</tr>
</tbody>
</table>
Modeling of Heat Release and Relevance of Ignition Delay

Wiebe’s function is widely used to characterize the heat release process for diesel engines. [84-86, 95, 96] Parameters in Wiebe functions need to be calibrated to match experimental data. Once matched, the Wiebe model can be a powerful tool for cycle simulation over the full operating range. However, prior to a detailed analysis of heat release profiles, it is critically important to distinguish between combustion modes, since multiple Wiebe functions are necessary for capturing typical features of diesel engine burn rates. As shown in Figure 3.14, some injected diesel fuel evaporates during the ignition delay period and burns in a premixed mode. This is followed by the mixing controlled, slower burning of the remaining fuel. Predicting the ratio of the two has profound impact on the shape of heat release profile. The heat release shape of diesel-only combustion is closely related to the distribution between premixed and mixing controlled burn stages, and knowledge of premixed fraction is critical for ensuring predictability of the Wiebe model.
Two Double-Wiebe function heat release correlations, developed by Watson[85] and Miyamoto[86], have been widely applied on conventional diesel engines in the past. Watson’s model separates diesel heat release into premixed and diffusion phases via Equation (3.16), where $m_{fb}$ is mass fuel burned, $m_{ft}$ is total fuel mass, $\beta$ is the premixed fraction used to quantify the mass-based ratio of fuel burned in premixed combustion to the total fuel, and $cw_1, cw_2, cw_3, cw_4$ are shaping factors. In Equation (3.16), $\tau_w$ is crank angle from onset of ignition normalized by total combustion duration $\Delta \theta_{cm,b}$, as given in Equation (3.17), where $\theta_{ign}$ is crank angle at onset of ignition. The premixed fraction $\beta$ is a function of ignition delay and equivalence ratio, where $a_w, b_w$ and $c_w$ are coefficients determined empirically.

$$\frac{m_{fb}}{m_{ft}} = \beta \left[ 1 - \left[ 1 - \tau_w^{cw_2} \right]^{cw_1} \right] + (1 - \beta) \left[ 1 - \exp \left[ -c_w \tau_w^{cw_4} \right] \right]$$  \hspace{1cm} (3.16)
Miyamoto’s Double-Wiebe model also divides heat release of diesel combustion into premixed and mixing control stages as given in Equation (3.19), both fitted with Wiebe functions, where $i = p, d$ stands for premixed and diffusion combustion stages, respectively, $\theta_{ign}$ is crank angle at onset of ignition, $\Delta \theta_i$ is combustion duration for premixed and diffusion combustion, $m_i$ is shape tuning factor and $Q_i$ is weighting factor to adjust heat release distribution between premixed and diffusion combustion stage. The sum of weighing factor should be equal to unity, as given in Equation (3.20).

\[
\frac{m_{pb}}{m_{bd}} = \sum_{i=p,d} Q_i \cdot \left\{ 1 - \exp \left[ -6.9 \left( \frac{\theta - \theta_{ign}}{\Delta \theta_i} \right)^{m_i+1} \right] \right\} \tag{3.19}
\]

\[
Q_p + Q_d = 1 \tag{3.20}
\]

Both Watson’s and Miyamoto’s correlations allow a reasonably good fitting of heat release for a conventional diesel engine, but both models fail to adequately address the tail of combustion. [97]

In the present work, an improved Triple-Wiebe function is developed and used to characterize both diesel-only and dual-fuel operation. The approach is similar to that proposed by Watson and Miyamoto, but a Triple-Wiebe function enables capturing of three heat release stages: Premixed, Main and Tail. The main and tail stages comprise the diffusion combustion stage. In the case of diesel-only combustion, the premixed
combustion stage represents the heat release contribution from fuel which became well mixed during the ignition delay period. Addition of tail combustion enhances late combustion fitting accuracy. The mathematical representation of Wiebe function for each stage remains the same as Miyamoto’s Double-Wiebe function, while Watson’s model in Equation (3.18) estimates heat release contribution from premixed combustion.

Therefore, the Triple-Wiebe function is given as:

\[
\frac{m_{fb}}{m_{fi}} = \sum_{i=p,m,t} f_i \left( 1 - \exp \left( -6.9 \left( \frac{\theta - \theta_{ign}}{\Delta \theta_i} \right)^{m_i+1} \right) \right)
\]

(3.21)

where \(i = p, m, t\) stands for premixed, main and tail combustion stages, respectively, \(\theta_{ign}\) is crank angle at onset of ignition, \(\Delta \theta_i\) is combustion duration for premixed, main and tail combustion, \(m_i\) is shape tuning factor, and the sum of each stage should be equal to the total heat release:

\[
f_p + (f_m + f_t) = 1
\]

(3.22)

Here main and tail factors \(f_m, f_t\) are grouped to represent mixing-controlled combustion. The premixed factor \(f_p\) is defined following Watson’s concept. The length of delay period determines how well the diesel spray evaporates and mixes with surrounding air, which directly affects the amount of fuel burned in premixed combustion, as illustrated in Figure 3.14. Hence, the premixed fraction of baseline diesel combustion is determined according to Equation (3.18). Watson suggested following ranges for adjustable parameters \(a_w, b_w\) and \(c_w\):

\[
0.8 < a_w < 0.95; \quad 0.25 < b_w < 0.45; \quad 0.25 < c_w < 0.5;
\]

(3.23)
Total number of 33 sets of experiment data were used in the effort of selecting optimal combination of $a_w$, $b_w$ and $c_w$. The Double-Wiebe approach was used first to manually fit the experiment heat-release profile and weighing fraction of premixed burn was recorded. A parameter sweep was conducted with Equation (3.18) with ranges given in (3.23) 0.95, 0.25 and 0.25 for $a_w$, $b_w$ and $c_w$ yielded premixed fractions that correlate best with the fitting results across operating points. Figure 3.15 shows the trend of premixed fraction with ignition delay and equivalence ratio. Experiment data with diesel-only operations from 1000 to 2000rpm with IMEP ranging from 5 to 25 bar were used to calibrate the Triple-Wiebe model. The Wiebe parameters used in this calibration process are shown as scattered points in Figure 3.16. It was discovered that Wiebe parameters are not showing strong dependency to engine speed. Linear correlations between Wiebe parameters and engine load (IMEP) were inferred from the calibration, which is also shown in Figure 3.16. A summary for selection of Wiebe parameters is given in Table 3.5. Premixed fraction $\beta$ is calculated from Equation (3.18). The shaping and duration factors for premixed and main stages are given as a linear function of engine load, while Tail shaping factor and tail fraction are constant.
Figure 3.15. Premixed fraction as a function of ignition delay and equivalence ratio, diesel-only case
Figure 3.16. Triple-Wiebe function parameters as a function of engine load.

Table 3.5. Selection of Triple-Wiebe function parameters

<table>
<thead>
<tr>
<th></th>
<th>$m$</th>
<th>$\Delta \theta$</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Premixed</td>
<td>$m_P = -0.040IMEP + 1.87$</td>
<td>$\theta_P = -0.416IMEP + 9.97$</td>
<td>$\beta$</td>
</tr>
<tr>
<td>Main</td>
<td>$m_M = 0.016IMEP + 0.92$</td>
<td>$\theta_M = 0.909IMEP + 12.30$</td>
<td>$0.8 - \beta$</td>
</tr>
<tr>
<td>Tail</td>
<td>$m_T = 1.5$</td>
<td>$\theta_T = 0.655IMEP + 42.73$</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Results and Analysis

Model Validation: Diesel Only Condition
Figure 3.17 shows the application of Triple-Wiebe function to baseline diesel combustion. The three cases in Figures 12a-12c depict low load, medium load and high load at various engine speeds. Correlation captures the features of diesel only combustion very well, as fitting accuracy at the tail portion is greatly improved compared to original Watson’s or Miyamoto’s models, as shown in Figure 3.18. In Figure 3.17, with increase of engine load, a reduction of premixed fraction is observed and combustion duration is extended.
Figure 3.17. Experimental vs. Triple-Wiebe heat release, diesel-only case: a) low load, 1000 RPM, b) medium load, 1200 RPM, and c) high load, 1600 RPM. Premixed fraction is shown in the legend.

Figure 3.18. Comparison Double-Wiebe and Triple-Wiebe based methods for reconstruction of the heat release rate. 1200RPM, IMEP 15.5bar.
Figure 3.19 shows the comparison between the experiment and simulated normalized heat release rate (HRR), cumulative heat release and the relative error of cumulative heat release. The engine operated in dual-fuel mode at 1600 rpm with IMEP of 24 bar. NG substitution rate was 34% on an energy basis. The Wiebe function captured the three stages of heat release and matched experimental behavior well. The error analysis shows the error between the calculated and experimental cumulative heat release rate is less than 5% after 5 ATDC, diminishing to <1% in the late stages of combustion. The error is large only at the very the start of heat release, when the experimental heat release is close to zero. Typical ranges for the Wiebe shaping factors are suggested in Table 3.6.

![Figure 3.19: Experimental and Wiebe function predicted heat release profile](image-url)
Table 3.6: Suggested range of Wiebe shaping factors

<table>
<thead>
<tr>
<th></th>
<th>$m_i$</th>
<th>$a_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Premixed</td>
<td>[1.2  2.0]</td>
<td>[0.6  1.2]</td>
</tr>
<tr>
<td>Main</td>
<td>[1.5  2.5]</td>
<td>[0.3  1.0]</td>
</tr>
<tr>
<td>Tail</td>
<td>[1.0  1.3]</td>
<td>[1.1  1.5]</td>
</tr>
</tbody>
</table>

Variations of heat release characteristics when switching from diesel-only to dual-fuel combustion are captured through calibration of the Wiebe function, as seen in Figure 3.20. The engine operated at 1200 rpm with 12 bar IMEP. It is observed that dual-fuel combustion tends to exhibit a reduced premixed burning fraction due to the reduced diesel fuel quantity. The duel fuel operation also produces a longer ignition delay due to presence of NG during the mixture process [4]. The peak heat release rate of dual-fuel combustion is slightly higher and main combustion duration is shorter than diesel-only mode. The faster burn rate is contributed by multi point ignition of NG and subsequent simultaneous combustion of diesel and NG.

Figure 3.20: Diesel-only vs. Dual-fuel Heat release rate
Figure 3.21 compares predicted and measured cylinder pressures at engine speed of 1200 rpm and two engine loads, 12 bar and 17 bar respectively. The model provides an
accurate prediction of cylinder pressure for both diesel and dual-fuel mode. The effect of heat release from the combustion and heat transfer to the wall are captured. The dual-fuel combustion reduces the peak cylinder pressure due to the longer ignition delay that retards combustion. The compression pressure is lower too, due to a difference in turbocharger performance.

Previous section has established the methodology for SOI determination, ignition delay prediction and heat release analysis using a baseline diesel case. Similar procedure can be applied to dual-fuel combustion. Introduction of NG adds complexity to analysis, since the equivalence ratio cannot be simply defined as in the case of baseline diesel combustion. In addition, NG will burn in a premixed mode rather than diffusion mode, and this will be addressed in the latter part of this section.

In the present work, two separate definitions of equivalence ratio are applied: total equivalence ratio and pseudo-diesel equivalence ratio. The total equivalence ratio stands for the ratio of the fuel-to-oxygen relative to stoichiometry, where both diesel and NG are summed up as fuel, i.e.:

$$\phi_{total} = \frac{m_{\text{fuel}} / m_{O_2}}{\left( \frac{m_{\text{fuel}} / m_{O_2}}{st} \right)}$$

where $\phi_{total}$ is total equivalence ratio, $m_{\text{fuel}}$ is the total mass of diesel fuel and NG, $m_{O_2}$ is the mass of available oxygen in the cylinder charge and $\left( \frac{m_{\text{fuel}} / m_{O_2}}{st} \right)$ is the stoichiometric fuel-to-oxygen ratio, defined as:
\[
\left( \frac{m_{\text{fuel}}}{m_{O_2}} \right)_{st} = \frac{m_D + m_{NG}}{3.045 \cdot m_D + 3.612 \cdot m_{NG}}
\]  
(3.25)

where \( m_D \) is the mass of diesel and \( m_{NG} \) is the mass of NG. The constants 3.045 and 3.612 are stoichiometric oxidizer to fuel ratio for diesel and NG, respectively. Inclusion of NG in the cylinder charge displaces fresh air and thereby, the diesel spray is subject to lower oxygen levels than in case of baseline diesel operation. Hence another equivalence ratio needs to be defined to depict the conditions experienced by the diesel fuel in the cylinder charge. The pseudo-diesel equivalence ratio is defined as the ratio of the diesel-to-oxygen relative to the stoichiometric diesel-to-oxygen ratio:

\[
\phi_{pD} = \frac{m_D / m_{O_2}}{0.328}
\]  
(3.26)

where 0.328 is stoichiometric diesel-to-oxygen ratio. An inherent assumption is made that the diesel fuel has access to all the oxygen in the cylinder charge. The starvation effect NG has on oxygen is neglected, at least initially. Figure 3.22 shows a comparison of total equivalence and pseudo diesel equivalence ratio in the dual-fuel combustion cases investigated experimentally. NG substitution becomes knock limited at higher loads, leading to the increased pseudo-diesel equivalence for higher loads.
Analysis of dual-fuel ignition delay follows the same procedure detailed in the previous section. The delay period in dual-fuel combustion is defined as the time from start of diesel injection to the onset of combustion. Injection timing of diesel fuel is obtained from the timing and metering pulse measured experimentally.

The ignition delay correlation given in Equation (3.12) is modified for the dual-fuel combustion case. Instead of using total equivalence ratio defined in Equation (3.24), the pseudo diesel equivalence ratio given in Equation (3.26) is used. The modified correlation is given in Equation (3.27), where $E_a/R_a$ is with the same value as given in Equation (3.12) and gas temperature is calculated as given in Equation (3.5) with $\gamma$ of 1.35.
\[ \tau_{id} = 2.4 \phi_{pD}^{-0.2} \bar{P}^{-1.02} \exp \left( \frac{E_u}{R \bar{T}} \right) \]  \hfill (3.27)

Figure 3.23 shows the comparison of experimental and calculated ignition delay in the dual-fuel engine. It is shown that modified ignition delay correlation provides a good prediction, while the calculation based on the total equivalence ratio causes underestimation. The observed dual-fuel ignition delay is longer than the baseline diesel-only combustion at same engine speed and load, as shown in Figure 3.24. Due to the altered chemical properties of the cylinder charge that includes NG, and reduced diesel/O2 ratio.

Figure 3.23. Dual-fuel ignition delay calculated based on pseudo diesel equivalence ratio and total equivalence ratio vs. experimental ignition delay
Figure 3.24. Comparison of ignition delay between diesel only and dual-fuel operation at two engine speeds.

Figure 3.25 shows the application of Triple-Wiebe function to dual-fuel combustion. Instead of calculating the premixed fraction using Equation (3.18) applied in the baseline diesel-only combustion, a curve fitting using Triple-Wiebe function is applied first to characterize the distribution of each combustion stage. As shown in Figure 3.25, two cases with high and low NG substitution rate were examined. The first case with 65.6% NG substitution rate displays a high amount of premixed combustion (60 percent of total heat released), a value beyond the reasonable range of premixed fraction in the typical diesel only combustion. The second case is a higher load point, with a lower NG substitution rate of 34%. The heat release profile indicates an intense and fast heat release stage in the beginning, followed by a slower heat release stage coming afterwards.
Clearly, dual-fuel combustion is displaying different combustion characteristics than the baseline diesel combustion. A direct relationship between premixed fraction and NG substitution is present, namely, high premixed fraction at high NG substitution rate and a relatively lower premixed fraction at low NG substitution rate. Karim et al. [66]
believed the heat release of pilot injected dual-fuel combustion can be split into three stages. The first heat release stage is contributed by the combustion of pilot diesel fuel, meanwhile NG around the immediate vicinity of diesel spray is ignited at multiple points simultaneously, which is considered a second heat release stage. The second stage features a short duration and high heat release rate because of simultaneous ignition of NG at multiple points. The third and last stage of heat release is contributed by the turbulent flame propagation of the remaining NG. This explains the high premixed fraction shown in the first case in Figure 3.25, where the “premixed” stage of heat release represents the sum of both diesel premixed combustion and multi-site NG ignition.

In Karim’s theory, diesel combustion only contributes to the very first stage of heat release because only a low quantity diesel pilot injection is used. However, the dual-fuel application in the present work has NG substation rates between 30% and 65%. Thus, diesel fuel plays an essential role in both initial heat release and subsequent diffusion burn. To accommodate this difference, the heat release is split into four stages. As shown in Figure 3.26, the first stage (A) is the premixed combustion of diesel fuel following diesel injection and subsequent ignition delay. The second stage (B) is contributed by the mixing controlled diesel combustion and stage (C) is the multi-site ignition of NG near the vicinity of the combusting diesel fuel. The fourth stage (D) is from the flame propagation and possible auto ignition of remaining NG.
An assumption is made that combustion stage (A) follows the same correlation defined in Equation (3.18), but the diesel to oxygen equivalence ratio is substituted with pseudo diesel equivalence ratio defined in Equation (3.26). The heat release of diesel combustion is first determined with a Triple-Wiebe function. Ratio between premixed and mixing controlled burning is critical for achieving high accuracy of predictions; therefore, Watson’s correlation given in Equation (3.18) is applied. It captures the physical effect of ignition delay and pseudo-$\phi$ on the premixed burning fraction. The heat release profile of NG combustion can then be inferred by subtracting heat release contributed by diesel combustion from the total.

The resulting profile can be represented with another Triple-Wiebe function, and the outcome will provide insight into the nature of NG burning. Rather than using a correlation for premixed burning of diesel, a multi-site ignition of NG is considered, and a weighting factor is determined empirically from curve fitting. Completing this exercise

Figure 3.26. A schematic description of heat release stages of dual-fuel combustion.
sets the stage for dual-fuel combustion studies with a dual Triple-Wiebe – see Figure 3.27. Two Triple-Wiebe functions are applied to characterize heat release from diesel and NG combustion, respectively. For each case, the left figure shows total experimental heat release, as well as the diesel and NG contributions to the heat release. The right figure further breaks down the diesel and NG contributions into the four discrete combustion stages: premixed diesel, multi-site NG ignition, mixing controlled diesel combustion and NG flame propagation.

Four unique engine operating conditions are analyzed. Figure 3.27 (a) shows high substitution rate and medium load; Figure 3.27 (b) shows low substitution rate and high load; Figure 3.27 (c) shows high substitution rate and medium load and Figure 3.27 (d) shows low substitution rate and low load. Combustion starts with premixed combustion of diesel fuel, follows by the multi-site NG ignition, then the diffusion combustion of remaining diesel fuel and flame propagation of remaining NG. After the onset of diesel premixed combustion, NG entrained into the diesel burning zone is ignited, along with ignition of gaseous fuel at the vicinity of the flame, where high temperatures and higher NG local equivalence ratio was present (burning diesel has decreased locally available oxygen).
Figure 3.27. Separated diesel and NG heat release rate at different NG substitution rates, dual-fuel case
Figure 3.28 shows the mass fraction burned (MFB) in one dual-fuel combustion case. For a comparison of burn rates between each fuel, diesel and NG MFB normalized by the respective total quantities. Initially, diesel fuel contributes most of the heat release, followed by a rapid combustion of NG. Both fuels burn slowly towards the end of combustion.

Figure 3.28. Mass fraction burned, dual-fuel case. Individual fuels are normalized by their own total quantities separately.

Figure 3.29 shows multi-site NG ignition fraction as a function of NG substitution rate and NG equivalence ratio. Decreasing trend of multi-site NG ignition fraction is observed as either NG substitution rate or NG equivalence ratio increases. For both low NG substitution rate and low NG equivalence ratio cases, a larger percentage of NG energy is released during multi-site NG ignition. These cases typically exhibit a high quantity of premixed diesel heat release due to the large quantity of diesel injected. This provides a stronger ignitions source for NG. Also at very low NG substation rates, flame propagation becomes unstable due to the over-lean mixture.
Figure 3.29. Multi-site NG ignition as a function of (a) NG substitution rate by energy content (b) NG equivalence ratio
Dual-fuel Transient Analysis

During tests on the chassis dyno and the road, the driver experienced a lag in power delivery under transient load conditions when the engine was operating in dual-fuel mode. During a tip-in, or load increase at constant engine speed, the engine did not exhibit the same response as when operating on diesel fuel only. Similar behavior was observed at tip-out, or a load decrease at constant engine speed. It was hypothesized that the location of the NG injector upstream of the intake manifold created a transport delay of NG during transient operation. This NG transport delay is substantially longer than the almost instant response of traditional diesel injection quantity.

Figure 3.30 shows the NG transport delay predicted with GT-Power simulation. The engine operated at 1400 rpm in dual-fuel mode. A step increase in engine load from 6 to 16 bar IMEP occurred at t = 1s and NG command increased from 3 g/s to 9.6 g/s. The solid and dashed lines show the NG fraction just after the injector (upstream) and just before the intake valve (downstream). As hypothesized, the NG undergoes a transport delay, creating a disparity between upstream and downstream NG mass fractions. The decreasing trend of NG mass fraction after it reached its peak is attributed to gradual increase in boost during the turbo lag period.
Figure 3.30: NG transport delay

Figure 3.31: NG transport delay cylinder to cylinder variations

Figure 3.31 shows the cylinder to cylinder variation due to the NG transport delay. The variation is caused by the combined effect of: the relative position of each cylinder to NG injector, asymmetric geometry of the intake plenum-manifold junction and the cylinder firing order. However, the averaged NG mass fraction of each cylinder, which is shown in solid line, clearly represented the trend of the transport delay. A similar trend was observed at tip-out conditions.

To investigate the sensitivity of the NG transport delay to various engine conditions, a parameter sweep was carried out using the GT-Power simulation. Figure
3.3.2 shows the sweep of NG injection rate and engine RPM. The NG injector was commanded to deliver 4 g/s, 6 g/s and 8 g/s, respectively. It was found out that the transport delay was only a function of engine speed. The linear regression fit of the delay period as a function of engine speed is given in Figure 3.33.

The NG transport delay at tip-in/ tip-out can be mitigated by manipulating the diesel injection profile. During a tip-in, the diesel injector can be commanded to inject an extra amount of fuel for a short period time, and then gradually reduce the diesel injection back to the to the steady state amount at the new engine load condition. The diesel fuel injection amount during the tip-in period is defined as compensated diesel fuel mass. The compensated diesel mass is calculated based on the fuel energy content via equation (3.28).

\[ m_{D_c} = \frac{E_{T_2} - E_{NG}}{E_{D_1}} \cdot m_{D_1} \]  

(3.28)

where \( m_{D_c} \) is the compensated diesel fuel mass, \( E_{T_2} \) is the total energy content of NG and diesel fuel after tip-in. \( E_{NG} \) is the energy content of NG before tip-in. \( E_{D_1} \) is the energy content of diesel fuel before tip-in. \( m_{D_1} \) is the injected diesel mass before tip-in.

Figure 3.34 shows a case of compensating the NG delay using the diesel injection. The simulation parameters are given in Table 3.7. The transient step increase of engine load demand occurred at \( t = 1s \). The NG was commanded to inject at a rate 3 times of the former steady state condition. A transport delay period was observed as shown in the top figure. To compensate this delay, at \( t = 1s \), the diesel injector was commanded to inject diesel fuel at a rate of 194\% of steady state diesel injection rate at \( t >1s \), which is shown
in the middle figure. The diesel injector maintained this rate for a short period of time and then linearly dropped back to the new steady state. According to the simulation results, the optimum duration of diesel injection compensation is to stay at $m_{Dc}$ for $1/3$ to $1/2$ of the NG transport delay duration. The bottom figure gives the compensation results. It was observed that the compensated diesel fuel injection effectively mitigated the NG transport delay. An IMEP comparison between the compensated results and diesel-only operation revealed that the compensation method achieved almost the same response. No torque dip or overshoot occurred.
Figure 3.32: NG mass fraction vs. engine speed, for three different NG injection rates
Table 3.7: Simulation parameters

<table>
<thead>
<tr>
<th></th>
<th>$t &lt; 1s$</th>
<th>$t &gt; 1s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine speed</td>
<td>1400rpm</td>
<td>1400rpm</td>
</tr>
<tr>
<td>IMEP demand</td>
<td>8 bar</td>
<td>15.5 bar</td>
</tr>
<tr>
<td>NG substitution rate</td>
<td>40%</td>
<td>60%</td>
</tr>
<tr>
<td>NG flow rate</td>
<td>2.7 g/s</td>
<td>8.2 g/s</td>
</tr>
<tr>
<td>Diesel injection rate</td>
<td>61.15 mg/cycle</td>
<td>82.49 mg/cycle</td>
</tr>
</tbody>
</table>
Figure 3.34: Diesel injection compensation of tip-in

One concern related to the diesel compensation method is that the instantaneous fuel injection amount may exceed the max injection capability of the diesel injector. Using equation (3.28), the compensated injection mass is calculated based on the fuel energy content. Since the energy content of compensated diesel fuel is calculated as $E_{T_2} - E_{NG_1}$, the fuel needed during compensation is less than the diesel injection amount in diesel-only mode, as shown in Figure 3.35. Hence the compensation will work at all load conditions without exceeding the capacity of the diesel injector.

Another concern is the transient emissions caused by the sudden increase of diesel injection. The transient diesel emission characteristics during a tip-in have been studied by Hagena et.al [98], where a drastic increase of soot emission was found to come along
with a step increase of engine load. In the dual-fuel case, an increase of soot emission will be expected too. However, as shown in Figure 3.35, the increased diesel injection quantity while utilizing the compensation algorithm in dual-fuel mode is still considerably smaller than the change in injected diesel mass during diesel-only operation. Hence, the problem with soot spikes should not be as severe, as the NG gas surrounding the sprays is well mixed and burns relatively clean.

![Comparison of injected diesel mass](image)

**Figure 3.35: Comparison of injected diesel mass**

The compensation algorithm for tip-out conditions is similar to tip-in with a few exceptions. According to equation (3.28), when the total fuel energy content after tip-out $E_T$ is smaller than the NG energy content before tip-out $E_{NG}$, the compensated diesel injection quantity becomes negative, which is forced to zero. This behavior is exhibited by Figure 3.36, where the compensated diesel injection bottoms out at zero. This physical constraint on the minimum diesel injection still results in improved tip-out IMEP matching, but the compensation result was not as good as the diesel-like response observed in tip-in cases.
Conclusions

This work has presented development of a phenomenological combustion model of a heavy-duty, dual-fuel engine, aided by insights from experimental data. Results characterize dual-fuel heat release in an engine where diesel fuel plays a significant role rather than simply acting as an ignition source for the gaseous fuel. The NG substitution rates vary between 30%-60%.

A Triple-Wiebe combustion model is developed to represent the heat release profile of both diesel-only and dual-fuel operation. It improves the fidelity of predictions compared to a typical Double-Wiebe model, particularly the 50%-100% burned phase. Accurate ignition delay predictions are enabled through application of a pseudo-diesel equivalence ratio. Calibration of constants in the model is performed based on the
experimentally determined burn rates in a heavy-duty six-cylinder 15 Liter engine. Values of constants are provided for a range of engine loads and speeds. Engine was instrumented with cylinder pressure transducers, and liquid fuel injection timing was determined from the injector solenoid pulse signal. A special correlation was developed to enable SOI calculation without a needle lift sensor. This enabled development of an ignition delay correlation based on pseudo diesel equivalence ratio, and its subsequent validation under dual-fuel combustion operating conditions. This will be invaluable for development of the development of multi-zonal diesel spray-combustion model for dual-fuel engines pursued in Chapter 5.

The combustion analysis process discussed in this work will not provide a detailed quantification of combustion characteristics in terms of heat release rate. However, modeling dual-fuel combustion with Triple-Wiebe functions provides an opportunity to discern the nature of dual-fuel combustion. Heat release contributions from diesel and NG are separated over a range of engine operation and NG substitution rates. Overall, dual-fuel combustion is split into four stages: premixed diesel, mixing controlled diesel, multi-site NG ignition and NG flame propagation. Predicted diesel burn rates are subtracted from the total to yield NG energy release profile. This allows estimation of heat release distribution between multi-site ignition and flame propagation of NG. Multi-site NG ignition fraction tends to decrease with both higher NG substitution rate and NG equivalence ratio.

A detailed 1-D GT-Power model of a dual-fuel engine was also developed in this work. A triple-Wiebe combustion model was calibrated to accurately represent both
diesel-only and dual-fuel operation and was plugged in the GT-Power model. The combustion model, VGT behavior, intake and exhaust gas flow predictions, and gaseous fuel injection dynamics were validated against a comprehensive set of experimental data acquired on the fully instrumented HD engine.

A source of lag in power delivery under transient load with dual fuel operation was studied using the 1-D engine system simulation. In particular, the CNG transport delay is characterized, and it was shown that the lag in response can be traced back to NG transport delay. Insights were used to develop a compensation algorithm for tip-in/ tip-out transients. It was found that a dynamic compensation through increased diesel injection will effectively mitigate the power lag resulted from NG transport delay during tip-in. Under some tip-out conditions, the lag cannot be fully mitigated through manipulating diesel injection profile because of signal saturation, but the algorithm performs well for most conditions.
CHAPTER FOUR

QUASI-D SPRAY AND COMBUSTION MODELING OF DIESEL ENGINE

Introduction

Previous chapter has discussed the 0-D modeling work related to dual-fuel engines. To obtain more predictiveness and fidelity, spatial resolution is needed. Quasi-D models offer a balance between model fidelity and computation requirement, thus is favored for system level analysis and real-time applications. In an effort to develop a Quasi-D predictive combustion model for dual-fuel engines, the modeling approach of diesel spray and its combustion need to be addressed first.

In this work, a Quasi-D diesel combustion model which marries predictiveness and computational speed required for engine system analysis is developed. Quasi-D models for diesel engine cycle simulations have been studied by multiple research groups in many decades. One of the most comprehensive studies was pioneered by Hiroyasu and his group, where a framework of Quasi-D, multi-zonal diesel spray-combustion model was proposed[99, 100]. Other researchers have applied the same framework to the development of their combustion models or have improved some of the sub-models[101, 102]. As the modern diesel engine technology advances, some of the sub-models in the original framework no longer apply or fail to provide accurate prediction results, one of which is the spray penetration model[103, 104]. The diesel injectors used in Hiroyasu’s experiment for calibrating the spray tip penetration model were a lot different compared to modern injectors, in terms of injection pressure and injector hole diameters. This results in a discrepancy between the model predicted and experimental measurement
penetration length on a modern injector. Other issues such as the effect of EGR on the ignition and combustion characteristics also need to be address if the original modeling framework is to be applied with a modern engine.

The main objective of this work is to develop a Quasi-D multi-zone diesel engine cycle simulation tool that works with modern engines with high pressure injector and EGR. The modeling scheme is based on the framework developed by Hiroyasu et al., with several improvements on sub-models, including:

- Improved spray tip penetration model to accommodate the recent development of injectors.
- Modified Ignition delay correlation that captures the effect of oxygen concentration, to capture the effect of EGR.
- Additional rule in determining the heat release rate, where the chemical reaction rate of hydrocarbon oxygen mixture is included in the algorithm.
- Performance of newly developed models spray and combustion models was validated with experiments on a single-cylinder small diesel engine with common rail fuel injection, charge boosting, and EGR.

**Quasi-D Modeling of Diesel Combustion**

The combustion of a diesel engine is a mixing-controlled process [105]. After being injected into the cylinder at high pressure, the fuel evaporates, interacts with air and auto-ignites, while fresh fuel keeps entering the combustion chamber and reacting with surrounding air, fuel and burned products. Unlike the turbulent flame combustion
modeling widely used in SI engines where only two zones (burned and unburned) are assumed, Quasi-D modeling of diesel combustion requires more spatial resolution to achieve reasonable level of prediction accuracy. The fundamental methodology of multi-zone spray modeling proposed by Hiroyasu et al. divides the incoming fuel into multiple packets and tracks the evolution of each packet individually[100]. As shown in Figure 4.1(a), a spray is considered to consist of multiple slices perpendicular to the spray penetration direction, shown as Plane A. In each slice, the fuel mass is further divided into multiple packets along the Y and Z direction, as shown in Figure 4.1(b). Fuel mass is assumed to distribute evenly in the radial (Y, Z) direction.
Figure 4.1. Spatial illustration of spray modeling scheme – defining the packets.

Figure 4.2 further illustrates the definition of packets in the X-Z plane. Figure 4.2(a) shows the slices of spray in the X direction where fuel mass is further divided into multiple packets in Z direction. Each packet is referred as $P(i,j)$, where $i$ is the index of packet in X direction while $j$ is the index in Z direction. The mass of fuel in a packet group $P(i,:)$ is determined by the fuel injection rate, while the fuel mass of each packet $P(i,j)$ is distributed evenly in Z direction. Since fuel spray penetration in the periphery region is less than the spray center, the penetration length of each packet on Z direction varies with its radial distance to the centerline. Figure 4.2(b) further illustrates spatial geometry of spray packets where the difference in penetration length of each packet is considered. In the Quasi-D spray-combustion simulation developed in this work, it is assumed that mass and enthalpy transfer between outside and inside of the spray are allowed, while no transfer of heat or matter are allowed to occur between packets.
Figure 4.2. Definition of packets in a spray (X-Z plane).

Figure 4.3 shows a schematic description of the simulation process. The engine cycle simulation starts at intake valve closing (IVC) and ends at the exhaust valve opening (EVO), thus no mass transfer occurs between ambient and in-cylinder charge during the simulation span. The initial in-cylinder gas composition can be either air or the mixture of air and residual gas. In the compression stroke before start of injection (SOI), the thermodynamics model updates the in-cylinder temperature and pressure with consideration of heat loss to the wall. After SOI, fuel is injected into the cylinder which triggers the sub-models for calculating spray tip penetration, air entrainment and fuel evaporation. The spray tip penetration model estimates the penetration length of each packet, which serves as the input for the latter air entrainment and fuel evaporation calculations. In this work, a new spray tip penetration model is developed and implemented to address limitations in validity of the original models. The spray tip penetration calculation is followed by air entrainment and fuel evaporation calculations. The air entrainment model calculates the rate of air or air/EGR mixture entraining into each packet, while fuel evaporation model calculates the evaporation rate of fuel droplets and outputs fuel vapor mass in each packet. The outputs of air entrainment and fuel
evaporation sub-models provide information for calculating the heat release rate. The fuel injection event (SOI) also triggers a sub-model that calculates ignition delay. In this work, a new ignition delay correlation is proposed and implemented in the effort to capture the effects of EGR. The ignition delay model outputs the time between SOI and start of combustion (SOC). The ignition event then triggers sub-models for estimating heat release and NOx emissions. The heat release sub-model calculates the mass of fuel burned in each packet at each calculation step. This value is then translated to heat release rate on energy basis.

In the modeling framework proposed by Hiroyasu, two possible scenarios are considered in the heat release model: air entrainment controlled and fuel evaporation controlled, where heat release rate is determined by either available fuel vapor or air mass in the packet. This work proposes a third scenario, which is reaction rate controlled heat release rate. The third mode is introduced to capture the effect of EGR on the combustion rate. In parallel to the above mentioned models, the thermodynamics model runs in each calculation step to update gas composition and thermodynamic properties in each packet as well as the rest of cylinder charge. The thermodynamics model provides inputs for the NOx formation model and in-cylinder states for the next calculation step. The sub-models mentioned above will be discussed in detail in the latter sections.
Development of an Improved Spray Penetration Algorithm

As mentioned in the previous sections, the spray penetration model in the original spray-combustion simulations developed by Hiroyasu et al. fails to provide accurate prediction results due to the evolution of fuel injection systems over the years\[104\]. This work proposes an improved spray tip penetration algorithm that can be implemented in the existing framework. The development of the new algorithm is a joint effort with Hiroshima University. Here I would like to acknowledge professor Keiya Nishida for providing experimental data. Optical experiments were performed in a high-pressure,
high-temperature constant volume combustion vessel to aid development and validation of the new model. The experiment setup is shown in Figure 4.4.

The constant volume vessel is temperature and pressure controlled. An electric heater is installed in the bottom of the vessel to bring the in-vessel temperature to the same level as in a diesel engine. The injector used in the vessel is a piezo-actuated type, single-hole injector with hole diameter of 0.111mm. The injection pressure is controlled by a high-pressure generator. The injection mass, injection timing and the image recording timing were controlled by DG645 by setting the pulse lengths. The spray behavior was observed through a transparent quartz window. For Non-evaporating spray, images were captured by the high-speed video camera (Photoron Co., ultima FASTCAM-APX RS) with 10,000fps frame rate and 512×512 pixels resolution. In the case of non-evaporating spray, the image was captured with the high speed camera with the aid of xenon lamp and two reflection mirrors which serve as the source of scattering light. Before each experiment, a scale ruler was inserted into the constant volume vessel and scale image was taken by the high speed video camera with the same settings as used for experiments. Each experimental test was repeated at least three times, and spray tip penetration was measured at various injection pressures. The specifications of experimental setup and test conditions are summarized in Table 4.1.
Figure 4.4. Optical experiment setup for measuring spray tip penetration.

Table 4.1. Specifications of the modeled Pentastar 3.6L V6 engine.

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient gas</td>
<td>Air [21% O₂, 79% N₂]</td>
</tr>
<tr>
<td>Ambient pressure ( P_a ) [bar]</td>
<td>15</td>
</tr>
<tr>
<td>Ambient temperature ( T_a ) [K]</td>
<td>300</td>
</tr>
<tr>
<td>Ambient density ( \rho_a ) [kg/m³]</td>
<td>18</td>
</tr>
<tr>
<td>Fuel type</td>
<td>Diesel JIS2</td>
</tr>
<tr>
<td>Injector type</td>
<td>Piezo-actuated</td>
</tr>
<tr>
<td>Number of holes</td>
<td>1</td>
</tr>
<tr>
<td>Hole diameter [mm]</td>
<td>0.111</td>
</tr>
<tr>
<td>Injection pressure ( P_{inj} ) [bar]</td>
<td>1000, 1300, 1450</td>
</tr>
<tr>
<td>Injection quantity ( Q_{inj} ) [mm³]</td>
<td>5</td>
</tr>
</tbody>
</table>

The widely used spray tip penetration algorithm developed by Hiroyasu et al.[106] are given in Equations (4.1)-(4.3). The break up time \( t_b \) is a parameter to characterize the time between SOI and breakup of the fuel jet. Break up time is
represented as a function of injector hole diameter $d_0$ and pressure difference between injector and ambient $\Delta P$. After fuel is injected and before break up time is reached, spray tip penetration $S$ is a linear function of time $t$, as shown in Equation (4.2). After break up time, spray tip penetration is represented as a function of $\sqrt{t}$, shown in Equation (4.3).

$$t_b = 28.65 \frac{\rho_d d_0}{\sqrt{\rho_a \Delta P}} \quad (\text{4.1})$$

$$S = 0.39 \sqrt{\frac{2 \Delta P}{\rho}} t, \quad 0 < t < t_b \quad (\text{4.2})$$

$$S = 2.95 \left( \frac{\Delta P}{\rho_a} \right)^{1/4} \sqrt{d_0 t}, \quad t_b \leq t \quad (\text{4.3})$$

The longest penetration in the spray occurs in the spray centerline. In the periphery region of the spray, penetration length reduces as the location moves from the center to the outer region of the spray, as have been illustrated in Figure 4.2(b). The mathematical representation of spray penetration at periphery region of the spray is given in Equations (4.4) and (4.5), where $E_x$ is introduced as a weighting factor in the radial direction of the spray. The weighting factor $E_x$ is represented as a function of $x_d$, which is the non-dimensional radial distance from spray centerline. At the centerline of the spray, $x_d$ equals to 0 and $E_x$ is at its maximum value of 1, while at the outer region of the spray, $x_d$ equals to 1 and $E_x$ reaches its minimum value of 0.5. The break up time and penetration length at periphery region of the spray are represented as a function of $E_x$:

$$E_x = 0.5 \sqrt{1 - x_d} + 0.5 \quad (\text{4.4})$$
\[ t_{hu} = E_s t_b, \quad S_x = \sqrt{E_s S} \tag{4.5} \]

Figure 4.5 shows a comparison between experimentally measured spray tip penetration and penetration length predicted by Hiroyasu-Arai’s correlation[106]. The injection pressure was 1000 bar and ambient pressure was 15 bar in this test case. It is shown that the Hiroyasu-Arai model overpredicts tip penetration before spray break up and underpredicts after the break up. The model also underpredicts the break up time, which is the major cause for underprediction of tip penetration after break up. The discrepancy between experimental data and model prediction is likely due to the model calibration conditions. At the time when the Hiroyasu-Arai correlation was developed, the injectors used were quite different compared to modern designs. The injector nozzle hole diameters were larger, e.g. 0.3, 0.7 and 0.84mm in [99], in contrast to much smaller holes used in the experiments for this work (0.11mm). Additionally, the fuel injection pressures used in the original Hiroyasu’s study were 7, 10 and 15 MPa, which were again much lower than the typical conditions in modern engines (>100MPa). Thus, there is a need to develop the new sub-model suitable for studies of engines with modern injection systems.
Figure 4.5. Comparison between Hiroyasu-Arai spray tip penetration model and experimental data.

The correlation for calculating injection velocity and break up length in the Hiroyasu-Arai correlation are given in Equation (4.6), where $\alpha_v$ and $\alpha$ are velocity coefficient and break up time coefficient, respectively. These two coefficients are defined
as constants in the original Hiroyasu-Arai’s correlation as $\alpha_v = 0.39$ and $\alpha = 15.8$. New values for these two coefficients or new correlations need to be developed to account for the design of modern injectors and elevated injection pressures.

$$v_0 = \alpha_v \sqrt{\frac{2\Delta P}{\rho_i}}, \quad L_b = \alpha \sqrt{\frac{\rho}{\rho_a} d_0} \quad (4.6)$$

Kanno et al. proposed an improved correlation to address the inaccuracy issues associated with the Hiroyasu-Arai model\[104\]. Instead of using constant $\alpha_v$ and $\alpha$, these two coefficients are modeled as a function of ambient density to account for the effect of varying cylinder pressure conditions during the injection event. The $\alpha$ and $\alpha_v$ are calculated as given in Equation(4.7).

$$\alpha = 27 \left( \frac{\rho_a}{\rho_0} \right)^{-0.125}, \quad \alpha_v = 0.7 \left( \frac{\rho_a}{\rho_0} \right)^{-0.25} \quad (4.7)$$

The break up time, spray tip penetration before and after break up with new $\alpha$ and $\alpha_v$ are given in Equations (4.8)-(4.10).

$$t_b = 27 \left( \frac{\rho_a}{\rho_0} \right)^{0.125} \frac{\rho_0 d_0}{\sqrt{2\rho_a \Delta P}} \quad (4.8)$$

$$S = 0.70 \left( \frac{\rho_a}{\rho_0} \right)^{-0.25} \frac{2\Delta P}{\rho_i} \sqrt{t}, \quad 0 < t < t_b \quad (4.9)$$

$$S = 4.35 \left( \frac{\rho_a}{\rho_0} \right)^{-0.188} \left( \frac{2\Delta P}{\rho_a} \right)^{0.25} \sqrt{d_0 t}, \quad t_b \leq t \quad (4.10)$$

The constants used in Kanno’s correlation were calibrated with injection pressures up to 150MPa and injector hole diameters between 0.12 and 0.147mm. The prediction
results with Kanno’s model compared with experimental results are shown in Figure 4.6. It is shown that Kanno’s model gives better prediction results of break up time and break up length compared to Hiroyasu-Arai’s model. However, discrepancy exists between the calculation of penetration length when $t = t_b$. Equations (4.9) and (4.10) output different values at the break up time. After the spray break up, Kanno’s model greatly underpredicts spray tip penetration.
Figure 4.6. Comparison between Kanno’s spray tip penetration model and experimental data.

To address the aforementioned issues, some coefficients in Kanno’s model are modified to achieve consistency of penetration length calculation at $t = t_b$. Equations (4.11)-(4.13) give modified equations for $\alpha$, $t_b$ and tip penetration after breakup. The equations for $\alpha_v$ and tip penetration before break up remain the same as given in Equations (4.7) and (4.9).

\[
\alpha = 27 \left( \frac{\rho_a}{\rho_0} \right)^{-0.1}
\]

\[
t_b = 38.57 \left( \frac{\rho_a}{\rho_0} \right)^{0.15} \frac{\rho d_0}{\sqrt{2 \rho_a \Delta P}}
\]

\[
S = 4.347 \left( \frac{\rho_a}{\rho_0} \right)^{-0.175} \left( \frac{2 \Delta P}{\rho_a} \right)^{0.25} \sqrt{d_0 t}, \quad t_b \leq t
\]
Figure 4.7 shows comparison between experimentally measured spray tip penetration data and predictions of the improved model. It is shown that the new model achieves better predictions of both break up time and tip penetration after the break up compared to Kanno’s model. The improved model yields good overall results of spray break up time, break up length and tip penetration before and after spray break up.
Figure 4.7. Comparison between improved spray tip penetration model and experimental data.

The improved spray tip penetration model is further validated with additional sets of experimental data. Figure 4.8 shows validation results for two different injection pressures. The improved model demonstrates good agreement with experimental data in both cases and shows considerable improvement compared to the original Hiroyasu-Arai model. It is shown that the improved model overpredicts tip penetration after 0.5ms ASOI in both cases. This is likely due to the fact that spray penetration no longer follows the function of square root of time after a certain time. For diesel engine applications, the prediction accuracy of first 0.5ms after injection has most significance since the spray is likely to impinge on the wall afterwards.
Modeling of Fuel-air Mixing

After the fuel is injected into the cylinder, it starts to interact with the surrounding air immediately. This process consists of two major events: air entrainment and droplet evaporation. These two processes last through the entire combustion cycle and have critical impact on the combustion characteristics. Specifically, the mass of entrained air and evaporated fuel in each packet before autoignition determine the characteristics of premixed combustion, while air entrainment and fuel evaporation rates afterwards determines the characteristics of diffusion combustion, thus the modeling of fuel-air mixing, especially these two processes need to be carefully addressed.

Air Entrainment Model
The rate of air entrained into each packet is calculated according to the correlation developed by Hiroyasu and Arai [106], as given in Equation (4.14). Air entrainment rate is determined by the mass of fuel in the packet \( m_{f0} \), injection velocity \( v_0 \), fuel and air density \( \rho_f, \rho_a \), break up time coefficient \( \alpha \), radial weighting function \( E_x \), nozzle hole diameter \( d_0 \) and mass of air entrained into the packet \( m_a \). The ODE is updated in every calculation step to output mass of air entrained into the packet. The injection velocity is calculated as given in Equation (4.15), which is derived from the improved spray tip penetration model.

\[
\frac{dm_z}{dt} = \frac{2m_{f0}^2 v_0^2}{\sqrt{v_0} \left( \frac{\rho_f}{\rho_a} \right)^{1/4} \sqrt{\alpha E_x d_0 (m_a + m_{f0})}} \tag{4.14}
\]

\[
v_0 = 0.70 \left( \frac{\rho_a}{\rho_0} \right)^{-0.25} \sqrt{\frac{2\Delta P}{\rho_f}} \tag{4.15}
\]

Fuel Evaporation Model

After fuel is injected into the surrounding air or air-EGR mixture, it breaks into numerous small droplets. The diameter of the droplets has a critical effect on the evaporation rate of fuel. Hiroyasu et al. proposed to use Sauter mean diameter (SMD) to represent the distribution of fuel droplet size[107]. The distribution of SMD in each packet is assumed to be uniform. The calculation of SMD is given in Equations (4.16)-(4.18), where \( D_{32} \) is SMD, \( d_0 \) is nozzle hole diameter, \( \mu_f \) and \( \mu_a \) are viscosity of fuel and air, \( Re \) is Reynolds number and \( We \) is Weber number.
\[
\frac{D_{32}^{LS}}{d_0} = 4.12 \text{Re}^{0.12} \text{We}^{-0.75} \left( \frac{\mu_i}{\mu_a} \right)^{0.54} \left( \frac{\rho_i}{\rho_a} \right)^{0.18} \tag{4.16}
\]

\[
\frac{D_{32}^{HS}}{d_0} = 0.38 \text{Re}^{0.25} \text{We}^{-0.32} \left( \frac{\mu_i}{\mu_a} \right)^{0.37} \left( \frac{\rho_i}{\rho_a} \right)^{-0.47} \tag{4.17}
\]

\[
\frac{D_{32}}{d_0} = \max \left[ \frac{D_{32}^{LS}}{d_0}, \frac{D_{32}^{HS}}{d_0} \right] \tag{4.18}
\]

The Reynolds number \( \text{Re} \) and Weber number \( \text{We} \) used in the aforementioned equations are defined in Equations (4.19) and (4.20), where \( \text{Re} \) is a function of injection velocity \( v_0 \), nozzle hole diameter \( d_0 \) and kinetic viscosity of fuel \( \nu_i \); and \( \text{We} \) is a function of fuel density \( \rho_i \), injection parameters \( v_0, d_0 \) and surface tension of diesel fuel \( \sigma_i \).

\[
\text{Re} = \frac{v_0 d_0}{\nu_i} \tag{4.19}
\]

\[
\text{We} = \frac{\rho_i v_0^2 d_0}{\sigma_i} \tag{4.20}
\]

The evaporation rate of fuel droplets can be calculated once the distribution of droplet diameter is known. The fuel evaporation calculation scheme used in this work is from the work of Kadota et al[108]. The ODE to calculate evaporation rate of each droplet \( dm_i/dt \) is given in Equation(4.21), where \( D_i \) is the diameter of a fuel droplet, \( y_{A0} \) is the initial mass fraction of fuel in the packet and \( y_{A2} \) is the mass fraction of fuel vapor in the ambient gas.

\[
\frac{dm_i}{dt} = \pi D_i^2 k^* \frac{y_{A0} - y_{A2}}{1 - (1 + \zeta) y_{A0}} \tag{4.21}
\]
The value of \( y_{A2} \) is zero at the time when the fuel is injected. As liquid fuel evaporates over time, the \( y_{A2} \) is calculated as mass fraction of fuel vapor in the packet.

Mathematical representation of \( y_{A2} \) is given in Equation (4.22), where \( m_{fg} \) is the mass of fuel vapor in the packet and \( m_{p_{acg}} \) is the total mass of the packet in gaseous state.

\[
y_{A2} = \frac{m_{fg}}{m_{p_{acg}}} \tag{4.22}
\]

The \( \zeta \) in Equation (4.21) is the ratio between mass flux rate of ambient gas and fuel, which represents the effect of surface regression [107]. The definition of \( \zeta \) is given in Equation (4.23), where \( \rho_{p_{ac}} \) is the density of the packet, \( \rho_{l} \) is the density of liquid fuel and \( r_{l} \) is the radius of a fuel droplet.

\[
\zeta = -\frac{\rho_{p_{ac}}}{\rho_{l} + \frac{r_{l}}{3} \left( \frac{d\rho_{l}}{dt} + \frac{dr_{l}}{dt} \right)} \tag{4.23}
\]

The \( k^* \) in Equation (4.21) is the mass transfer coefficient, represented in the form of Equation (4.24), where \( \xi_{M} \) represents the effect of mass transfer on the mass transfer coefficient \( k^* \) and \( k \) is the mass transfer coefficient in the case of infinitesimal mass transfer [107]:

\[
k^* = \xi_{M} k \tag{4.24}
\]

where \( \xi_{M} \) is defined as a function of mass flux rate ratio, \( y_{A0} \) and \( y_{A2} \):

\[
\xi_{M} = \frac{1 - (1 + \zeta) y_{A0}}{(1 + \zeta) (y_{A0} - y_{A2})} \ln \left\{ \frac{1 - (1 + \zeta) y_{A2}}{1 - (1 + \zeta) y_{A0}} \right\} \tag{4.25}
\]
and \( k \) is represented as a function of Sherwood number \( Sh \), diffusivity of diesel fuel \( D_d \), packet density \( \rho_{pac} \) and droplet diameter \( D_i \):

\[
k = \frac{\rho_{pac} D_d \cdot Sh}{D_i}
\] (4.26)

The ODE for solving droplet diameter \( D_i \) is represented as a function of droplet diameter, density and mass, as given in Equation(4.27):

\[
\frac{dD_i}{dt} = \frac{2}{\pi D_i^2 \rho_i} \left( \frac{dm_i}{dt} - \frac{\pi D_i^3}{6} \frac{d \rho_i}{dt} \right)
\] (4.27)

With the diameter of fuel droplets known, the vaporized fuel mass in the packet \( m_{f,0} \) can be calculated as:

\[
m_{f,0} = \frac{\pi}{6} \left( \rho_{f,0} D_{f,0}^3 - \rho_i D_i^3 \right) N_D
\] (4.28)

where \( \rho_{f,0} \) and \( D_{f,0} \) are initial density and diameter of the fuel droplet and \( N_D \) is the total number of fuel droplets in the packet. The droplets number \( N_D \) is calculated as given in Equation(4.29), where \( m_{f,0} \) is the initial fuel mass in the packet.

\[
N_D = \frac{m_{f,0}}{\frac{4}{3} \pi \left( \frac{D_{f,0}}{2} \right)^3 \rho_{f,0}}
\] (4.29)

**Ignition Delay Model**

The ignition delay period in diesel engines is defined as the duration between SOI and SOC. Several correlations for predicting ignition delay have been proposed in the published work, including the Arrhenius function based correlations[85, 94, 109-111] and
chemical kinetics based models such as the Shell autoignition model[112, 113]. Among those approaches, the Arrhenius function based correlation developed by Assanis et al. has been widely used and proven to yield satisfying prediction results[94]. The correlation is represented as:

$$\tau_{ID} = 2.4 \phi^{-0.2} P^{-1.02} \exp\left(\frac{E_a}{R_u T}\right)$$  \hspace{1cm} (4.30)

where $\tau_{ID}$ is ignition delay in $ms$, $\phi$ is the equivalence fuel-air ratio, $P$ and $T$ are the cylinder pressure and temperature at SOI in bar and K and $E_a/R_u$ is constant 2100 for diesel fuel[85]. This correlation works very well for predicting ignition delay in diesel engines under both steady state and transient conditions. However, when an engine is equipped with EGR, which most of the modern diesel engines do, this correlation no longer gives a satisfying prediction of ignition delay since the dilution effect of the EGR is not included in this correlation.

In the effort of improving this ignition delay correlation to adapt for the inclusion of EGR, experimental data from a single cylinder research diesel engine was used to derive an improved correlation. The same experimental data was also used to validate the performance of the multi-zone diesel combustion model. Here I would like to acknowledge Kazuhisa Inagaki from Toyota for providing experimental data.

The research engine used in the experimental work is a single cylinder, turbo charged engine with direction injection. The injection system used was a G3P common rail system made by Denso and the injection scheme was single injection. Key features of the tested engine cranktrain and piston geometry are given in Figure 4.9, where $e$ is the
piston pin offset, \( l \) is the connecting rod length, \( r \) is crank radius and \( \delta \) is crankshaft offset. The geometries shown for the piston cavity shape are in mm. Specifications of the tested engine are summarized in Table 4.2. More information of the experimental test setup can be found in[114].

![Piston-crank Geometry and Piston cavity shape](image)

**Figure 4.9. Geometrical configuration of tested engine.**

**Table 4.2. Specifications of tested engine.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>mm</td>
<td>86</td>
</tr>
<tr>
<td>Stroke</td>
<td>mm</td>
<td>96</td>
</tr>
<tr>
<td>Connecting rod</td>
<td>mm</td>
<td>147.5</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>-</td>
<td>15.8</td>
</tr>
<tr>
<td>Top clearance</td>
<td>mm</td>
<td>0.71</td>
</tr>
<tr>
<td>Crankshaft offset</td>
<td>mm</td>
<td>10</td>
</tr>
<tr>
<td>Piston pin offset</td>
<td>mm</td>
<td>-0.25</td>
</tr>
<tr>
<td>Nozzle orifice diameter</td>
<td>mm</td>
<td>0.098</td>
</tr>
</tbody>
</table>
Two engine speed and load conditions with varying level of EGR were tested, the engine operating parameters for each tested cases are summarized in Table 4.3. The EGR ratio $X_{EGR}$ is defined as the mass fraction of EGR in the total mass of intake gas:

$$X_{EGR} = \frac{\dot{m}_{EGR}}{\dot{m}_{EGR} + \dot{m}_{Air}} \quad (4.31)$$

Table 4.3. Summary of engine test conditions.

<table>
<thead>
<tr>
<th>Low load</th>
<th>Engine Speed RPM</th>
<th>Target IMEP bar</th>
<th>Injected fuel mass mg/cycle</th>
<th>Injection pressure MPa</th>
<th>Injection timing deg ATDC</th>
<th>Intake temperature deg C</th>
<th>Boost pressure bar</th>
<th>EGR ratio %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1600</td>
<td>6.5</td>
<td>23</td>
<td>60</td>
<td>-3.3</td>
<td>40</td>
<td>1.1</td>
<td>0, 10, 16, 20, 24</td>
</tr>
<tr>
<td>High load</td>
<td>Engine Speed RPM</td>
<td>Target IMEP bar</td>
<td>Injected fuel mass mg/cycle</td>
<td>Injection pressure MPa</td>
<td>Injection timing deg ATDC</td>
<td>Intake temperature deg C</td>
<td>Boost pressure bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2000</td>
<td>16</td>
<td>54.8</td>
<td>180</td>
<td>4.5</td>
<td>40</td>
<td>2.0</td>
<td></td>
</tr>
</tbody>
</table>
The experimentally measured cylinder pressure for each tested case are shown in Figure 4.10. Measured cylinder pressure data was processed to derive apparent heat release rate (AHRR) using the scheme given in Equation (4.32) [33]:

$$\dot{Q} = \frac{\gamma}{\gamma - 1} P \dot{V} + \frac{1}{\gamma - 1} V \dot{P}$$

(4.32)

where $P$ is cylinder pressure, $V$ is instantaneous cylinder volume and $\theta$ is crank angle. The specific heat ratio $\gamma$ used in this equation is constant $c_p/c_v = 1.34$. The AHRRs derived from cylinder pressure data are shown in Figure 4.11. The crank angle shown in both figures are based on crank shaft position, and TDC is actually a “crank TDC”. Since there is an offset between the crankshaft and cylinder axes, the crank angle when piston reaches top dead position is retarded to 3 deg ATDC. Therefore, the true piston top dead-center corresponds to 3 deg ATDC. As can be seen from the cylinder pressure and AHRR profiles, for both low load and high load cases, increased EGR levels resulted in a prolonged ignition delay and lower peak cylinder pressure.
Figure 4.10. Cylinder pressure from experiment measurement. Two engine speed and load points are shown
The ignition delay is determined from the AHRR data as the period between SOI and SOC. Due to the measurement noise of cylinder pressure, the AHRR near SOC is quite noisy too. Thus, using the point where AHRR becomes positive as SOC is not
reliable. In this work, the SOC is determined as the point when HRR raises above 10J/deg.

The ignition delay correlation given in Equation(4.30) was first validated with experimental data. The prediction results from the correlation compared to experimentally derived ignition delay are given in Figure 4.12. It is shown that the predicted ignition delay drifts away from the experimental values as EGR ratio increases. Reduced oxygen concentration leads to a higher $\phi$, which according to Equation(4.30), results in a reduced ignition delay prediction. However, this is contradictory to the trend discovered in the experimental data. In reality, the inclusion of EGR reduces the cylinder gas temperature during the compression process, which in turn prolongs the ignition delay prediction.

![Figure 4.12. Comparison between the prediction results from existing ignition delay model and experimental data.](image)
From the results shown in Figure 4.12 it is clear that the correlation from [94] does not accurately predict ignition delay of diesel combustion with EGR. A new correlation is needed to account for the varying EGR levels. In this work, the ignition delay model from [94] is used as a basis, and more terms are added to provide required fidelity. The form of the new ignition delay correlation is given in Equation (4.33).

\[
\tau_{ID} = C_1 \phi^{-0.2} P^{-1.02} x_{O_2}^{C_2} \exp \left( \frac{E_a}{R \theta} \right)
\]  

(4.33)

In addition to the temperature, pressure and equivalence ratio at SOI, an additional parameter \(x_{O_2}\) which denotes oxygen mole fraction is included to capture the effect of EGR. The exponents for \(\phi\) and \(P\) remain the same as given in Equation (4.30).

Two constants \(C_1\) and \(C_2\) are the parameters to be determined from the fitting of experimental data, where \(C_1\) is ignition delay constant and \(C_2\) is the exponent of oxygen mole fraction. Since the \(\phi\) and \(P\) terms in the new correlation remain the same, the constants \(C_1\) and \(C_2\) can be fitted by using the experimentally determined ignition delay divided by the ignition delay predicted by the existing correlation, as given in Equation (4.34), where \(C_3 = C_1 / 2.4\).

\[
\frac{\tau_{ID, \text{exp}}}{\tau_{ID, \text{model}}} = C_3 x_{O_2}^{C_2}
\]  

(4.34)

A least square fit was applied to determine the coefficients \(C_2\) and \(C_3\) in Equation (4.34). Figure 4.13 gives the fitting results with experimental data. The y axis denotes the left side of Equation (4.34) and x axis is the mole fraction of oxygen. A clear trend of \(ID_{\text{exp}}/ID_{\text{model}}\) versus oxygen mole fraction is observed, which indicates the
existing model tends to underpredict ignition delay as oxygen mole fraction decreases. The coefficients acquired from the fitting are $C_2 = -1.87$ and $C_3 = 0.0466$, thus the coefficient $C_1$ in Equation (4.33) is determined as $C_1 = 0.11$.

![Figure 4.13. Least square fit of the ignition delay model coefficients.](image)

The modified ignition delay correlation with oxygen mole fraction included as an additional parameter is now determined in a form shown in Equation (4.35). Figure 4.14 shows its validation with experimental data, where the ignition delay predictions from both the existing and new models are shown. It is observed that the new model greatly improves ignition delay prediction accuracy compared to the baseline under varying EGR ratios.

\[
\tau_{ID} = 0.11\phi^{-0.2}P^{-1.02}x_{O_2}^{-1.87}\exp\left(\frac{E_a}{R_u T}\right)
\]  

(4.35)
Heat Release Model

In this work, it is assumed that in each packet, only fuel vapor reacts with surrounding air, while fuel droplets in liquid state are not consumed by combustion. The mass of fuel burned in a packet in each calculation step is determined by the mass of fuel vapor and air[100]. Equation(4.36) gives the scheme to determine the mass of fuel burned in each calculation step proposed by Hiroyasu et al. When the fuel vapor/air mixture is richer than stoichiometry, fuel mass burned $\Delta m_{\text{fuel}}$ is determined by the mass of air in the packet $m_a$ and stoichiometric air fuel ratio $AFR_{\text{stoich}}$. On the other hand, when the fuel vapor/air mixture is leaner than stoichiometry, $\Delta m_{\text{fuel}}$ is determined by the mass of fuel vapor $m_{fg}$. 

Figure 4.14. Comparison between the prediction results from improved ignition delay model and experimental data.
\[ \Delta m_{\text{fuel}} = \frac{m_a}{AFR_{\text{stoich}}}; \quad \phi > 1 \]
\[ \Delta m_{\text{fuel}} = m_{fg}; \quad \phi < 1 \]  \hspace{1cm} (4.36)

One limitation of this method is the combustion rate being determined exclusively by the available fuel or air mass in a packet. At each calculation step, either air or fuel is assumed to be entirely consumed. At conditions where the calculation time step is very small, or EGR is present in the mixture, this assumption does not hold very well. For the conditions with small calculation time steps, the existing scheme will yield a sharp spike of heat release rate at the premixed stage since all the air entrained into the packet and fuel vaporized during the ignition period would be consumed in a single timestep.

Additionally, for the conditions where EGR is present, the effect of reduced oxygen concentration from EGR on the burn rate cannot be captured. The same issue was also discovered by other researchers[102]. To address the aforementioned limitations, a third criterion is added in addition to what is given in Equation(4.36) to determine the mass of fuel burned in each calculation step:

\[ \Delta m_{\text{fuel}} = \dot{m}_{\text{chem}} \cdot \Delta t; \quad \Delta m_{\text{fuel}} > \Delta m_{\text{chem}} \]  \hspace{1cm} (4.37)

where \( \dot{m}_{\text{chem}} \) is the chemical reaction rate of hydrocarbon and oxygen mixture. When the mass of fuel burned at each calculation step determined from Equation(4.36) is smaller than \( \dot{m}_{\text{chem}} \Delta t \), the burn rate is determined from the result of Equation(4.36). In contrast, when the mass fuel burned at each step determined from Equation(4.36) is larger than the chemical reaction rate limit, the burn rate is determined by the output of Equation(4.37).

The chemical reaction rate of diesel-oxygen mixture can be determined from the following formula[79]:
\[ \dot{m}_{\text{chem}} = A_d \exp \left( -\frac{E_a}{RT} \right) [C_{12}H_{26}]^{0.25} [O_2]^{1.5} V_{\text{pac}} \cdot M_{\text{fuel}} \]  

(4.38)

where \( C_{12}H_{26} \) is used to approximate the chemical composition of diesel (n-dodecane), \( \dot{m}_{\text{chem}} \) is the chemical reaction rate of fuel in g/s, \( A_d \) is adjustable constant which is assumed as \( 2.5 \times 10^{10} \), \( E_a \) is activation energy with constant value of 30kcal/mol, \( R \) is universal gas constant in 0.001987kcal/mol/K, \( T \) is gas temperature in the packet in K, \( V_{\text{pac}} \) is packet volume in \( cm^3 \), \( M_{\text{fuel}} \) is the molecular weight of fuel in g/mol and \( [C_{12}H_{26}], [O_2] \) denote the concentration of fuel and oxygen in mol/cm\(^3\).

With this additional criterion, the effect of EGR on oxygen concentration is included, where decreased oxygen concentration will result in a lower reaction rate. Additionally, maximum mass of fuel that can be consumed at each calculation step is regulated, thus no more sharp spikes of heat release prediction at the initial stage of premixed combustion will be present. With this in mind, the total heat release rate from the combustion of fuel \( \dot{Q}_{\text{fuel}} \) is given in Equation(4.39), where \( LHV_{\text{fuel}} \) is the lower heating value of fuel and \( n_{\text{pac}} \) is the total number of packets.

\[ \dot{Q}_{\text{fuel}} = LHV_{\text{fuel}} \sum_{i=1}^{n_{\text{pac}}} \frac{\Delta m_{\text{fuel}}}{\Delta t} \]  

(4.39)

**Thermodynamics Model**

In this section, a thermodynamics model that runs in parallel with the sub-models given in the previous sections is given. The task of the thermodynamics model is to
update the pressure, temperature, composition and gas properties of each packet and the unburned gas in each calculation step. Pressure is of course uniform across the entire combustion chamber. In this work, mass transfer is allowed only from ambient to the spray packets while heat transfer is not allowed in both directions. The thermodynamics model also updates the bulk cylinder pressure and temperature and uses this information to calculate the heat transfer to the wall.

The cylinder pressure is uniform for both unburned gas zone and spray packets throughout the cycle. Equation (4.40) gives the ODE for updating cylinder pressure. The \( \gamma \) used in this correlation is updated in every calculation step as a function of temperature and gas composition. The calculation scheme for \( \gamma \) will be given in the latter section. The \( \dot{Q}_{\text{total}} \) is the heat input to the cylinder, obtained as the difference between the heat released from the combustion of fuel and heat loss to the wall, as given in Equation (4.41).

\[
\dot{P} = \frac{\gamma - 1}{V} \dot{\dot{V}}_{\text{total}} - \frac{\gamma}{V} P \dot{V} \tag{4.40}
\]

\[
\dot{Q}_{\text{total}} = \dot{Q}_{\text{fuel}} - \dot{Q}_{\text{ht}} \tag{4.41}
\]

In this work, the heat loss to the wall is obtained using the bulk cylinder temperature as input. It has been documented in the published work that the heat loss in a diesel engine consists of two major components: convective and radiative heat transfer, where radiative heat transfer can account for 20~30% of total heat transfer due to the oxidation of soot\[115, 116\]. Equation (4.42) defines the total heat transfer rate \( \dot{Q}_{\text{ht}} \) as the sum of convective heat transfer rate \( \dot{Q}_{\text{c}} \) and radiative heat transfer rate \( \dot{Q}_{\text{r}} \):
\[ \dot{Q}_{\text{all}} = \dot{Q}_c + \dot{Q}_r \] (4.42)

The convective heat transfer rate $\dot{Q}_c$ is obtained based on the widely accepted correlation proposed by Woschni et al.\[93\] Equation(4.43) gives the general form to calculate convective heat transfer, where $h_c$ is the Woschni convective transfer coefficient in $W/m^2 \cdot K$, $A_{\text{wall}}$ is wall area, including piston top, cylinder head and liner, $T$ is cylinder bulk gas temperature and $T_{\text{wall}}$ is the specified wall temperature. Due to the difference in temperature amongst piston, head and cylinder liner, heat transfer rate to each of these surfaces is calculated individually and summed up to arrive at the total. In this work, cylinder liner temperature is assumed as 400K while piston top and cylinder head temperatures are assumed to be 550K.

\[ \dot{Q}_c = h_c \sum A_{\text{wall}} (T - T_{\text{wall}}) \] (4.43)

The Woschni convective heat transfer coefficient $h_c$ in Equation(4.43) is given as the form of Equation(4.44), where $Bore$ is the cylinder bore diameter, $P$ is cylinder pressure, $T$ is cylinder bulk temperature and $w$ is the characteristic velocity. In this equation $P$ is in the unit of $kPa$ while all the rest parameters are in SI units. The characteristic velocity $w$ is defined in Equation(4.45), where $S_p$ is mean piston velocity, $P, V$ are instant cylinder pressure and volume, $T_r, \ P_r, \ V_r$ are cylinder temperature, pressure and volume at a reference state, $P_m$ is the motored cylinder pressure and $C_1, C_2$ are constants. In this work, intake valve closing is used as the reference state and $P_m$ is determined by using the adiabatic compression assumption. During the compression
stroke, \( C_1 = 2.28 \) and \( C_2 = 0 \), while during the combustion and expansion period, \( C_1 = 2.28 \) and \( C_2 = 3.24 \times 10^{-3} \). All parameters shown in Equation (4.45) are in SI units.

\[
h_e = 3.26 \text{Bore}^{-0.2} P^{0.8} T^{-0.55} W^{0.8}
\]

\[
w = C_1 S_p + C_2 \frac{V T_r}{P_r V_r} (P - P_m)
\]

The heat transfer from radiation is estimated as given in Equation (4.46), where \( \sigma = 5.67 \times 10^{-8} W m^{-2} K^{-4} \) is the Stefan-Boltzmann constant and \( \beta_r = 1.6 \) is adjustable constant[117]. Similar to what is given in Equation (4.43), the total radiative heat loss to the wall is the summation of the heat loss to the surface of piston top, cylinder head and cylinder liner.

\[
\dot{Q}_r = \beta_r \sigma \sum \left[ A_{wall} \left( T^4 - T_{wall}^4 \right) \right]
\]

An accurate estimation of gas temperature is critical for the combustion model, since the temperature would affect almost every aspect of the processes, including evaporation rate of fuel, chemical reaction rate of fuel-air mixture, estimation of ignition delay and prediction of temperature dependent emissions such as NOx. The temperature is calculated based on the expression derived from the application of the first law of thermodynamics described by Heywood[118]:

\[
\dot{T} = \frac{B'}{A'} \left[ \frac{\dot{m}}{m} \left( 1 - \frac{h}{B'} \right) - \frac{\dot{V}}{V} - \frac{C'}{B'} \phi + \frac{1}{B'm} \left( \sum_j \dot{m}_j h_j + \dot{Q}_w \right) \right]
\]

where:
In the above two equations, \( m \) is the mass in the control volume. When calculating cylinder bulk temperature, the total mass inside the cylinder remains constant since no mass transfer occurs while all valves are closed, thus the terms with \( \dot{m} \) are eliminated. However, when calculating the temperature in each packet and the unburned zone temperature, the change of mass in the control volume need to be considered. In Equation (4.47), \( V \) is control volume, \( h \) is the specific enthalpy of the gas in the control volume, \( \phi \) is the equivalence ratio, \( \sum \dot{m}_i h_i \) is the sum of enthalpy transfer rate and \( \dot{Q}_w \) is the heat transfer rate to the control volume. This equation applies to the calculation of cylinder bulk gas temperature, the temperature in each packet and the unburned gas temperature.

**Gas Composition and Property Model**

To implement the temperature model discussed above, a gas property model is needed to provide information of the composition of gas in the control volume and its physical properties such as the ratio of specific heats \( \gamma \) and enthalpy \( h \). In Equation (4.47), equivalence ratio \( \phi \) is used to incorporate the effect of gas composition on the temperature estimation. However, when the gas does not only consist of air and fuel,
using $\phi$ only will not have enough fidelity. Rather, a detailed gas property model is used
to estimate impact of gas composition, and the $\phi$ term is eliminated.

The gas composition and property model tracks the species of intake gas, burned
products and fuel in each control volume defined in the combustion model. The tracked
gaseous species include $O_2$, $N_2$, $CO_2$, $H_2O$ and diesel fuel vapor. The concentration of
$O_2$, $CO_2$ and $H_2O$ are determined from 1), the initial composition of gas, which is a
function of EGR ratio and composition of burned products, and 2), the chemical reaction
of diesel fuel and oxygen. Mathematical form of the gas property model for
$O_2, N_2, CO_2, H_2O$ is given in Equations (4.49) and (4.50), where specific heat capacity $c_p$
and enthalpy $h$ are represented as algebraic functions of the temperature in the control
volume. The coefficients $\alpha_1$ to $\alpha_6$ for each species are given in the Appendix A[119].

\[ \frac{c_p}{R} = \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \]  (4.49)

\[ \frac{h}{RT} = \alpha_1 + \frac{\alpha_2}{2} T + \frac{\alpha_3}{3} T^2 + \frac{\alpha_4}{4} T^3 + \frac{\alpha_5}{5} T^4 + \frac{\alpha_6}{6} \frac{1}{T} \]  (4.50)

For diesel vapor, the gas properties are obtained as:[33]

\[ \frac{c_p}{R} = \alpha_1' + \alpha_2' T + \alpha_3' T^2 + \alpha_4' T^3 + \alpha_5' \frac{1}{T^2} \]  (4.51)

\[ \frac{h}{RT} = \alpha_1' + \frac{\alpha_2'}{2} T + \frac{\alpha_3'}{3} T^2 + \frac{\alpha_4'}{4} T^3 - \alpha_5' \frac{1}{T^2} + \alpha_6' \frac{1}{T} \]  (4.52)

where coefficients $\alpha_1'$ to $\alpha_6'$ for diesel vapor are provided in Annex A. The temperature
used in the above gas property calculations are the gas temperature of the control volume.
Specific heat capacity $c_p$ is in unit of $J \cdot kg^{-1} K^{-1}$; specific enthalpy $h$ is in $J/kg$ and
specific gas constant $R$ is in $J \cdot kg^{-1} K^{-1}$. The specific gas constant $R$ is calculated from the composition of species in the control volume and heat capacity ratio $\gamma$ is calculated as a function of $R$ and $c_p$:

$$\gamma = \frac{c_p}{c_p - R} \quad (4.53)$$

Substitute Equations (4.49)-(4.52) to Equation(4.48), Equation (4.48) can be re-written as:

$$A' = c_p - \frac{P}{\rho T}, \quad B' = RT, \quad C' = 0 \quad (4.54)$$

Substitute Equation(4.54) to the temperature calculation scheme given in Equation(4.47), the partial differential terms are eliminated. The temperature in each control volume can now be updated through the ODE given in Equation(4.55), where $\gamma$, $h$ and $h_j$ are calculated from the above discussed gas property model.

$$\dot{T} = T(\gamma - 1) \left[ \frac{\dot{m}}{m} - \frac{\dot{m} h}{PV} - \frac{\dot{V}}{V} + \frac{1}{PV} \left( \sum_j \dot{m}_j h_j + \dot{Q}_w \right) \right] \quad (4.55)$$

**NOx Formation Model**

The NOx emission is a critical parameter in diesel engines as the exhaust emission regulation keeps tightening. Generally NO and NO$_2$ are grouped together to represent NOx emissions. For diesel engines, NO emission is dominant[33], thus this work will focus only on NO. The NO emission prediction scheme is based on the extended Zeldovich mechanism [120, 121], which consists of three major reactions:
\[ O + N_2 \rightleftharpoons NO + N \quad (1) \]
\[ N + O_2 \rightleftharpoons NO + O \quad (2) \]
\[ N + OH \rightleftharpoons NO + H \quad (3) \]

The chemical reaction rate constant of the three reactions are given in (4.57), where \( k_i^+ \) and \( k_i^- \) stand for forward and reverse rate constants in \( cm^3/mol \cdot s \), respectively. The subscript \( i \) corresponds to the reactions 1-3 defined in Equations (4.56).

It is obvious that the rate constants depend exclusively on the temperature, thus the NO formation model can also be used for validating the temperature prediction.

\[
k_i^+ = 7.6 \times 10^{13} \exp\left(-38000 / T\right) \\
k_i^- = 1.6 \times 10^{13} \\
k_2^+ = 6.4 \times 10^9 T \exp(-3150 / T) \\
k_2^- = 1.5 \times 10^9 T \exp(-19500 / T) \\
k_3^+ = 4.1 \times 10^{13} \\
k_3^- = 2.0 \times 10^{14} \exp(-23650 / T)
\]

Due to the low concentration of N, a steady-state approximation for the concentration of N is assumed, where \( d[N]/dt \) is set to zero throughout the reaction [120]. Under this assumption, the NO formation rate can be represented as:

\[
\frac{d[NO]}{dt} = 2k_i^+[O][N_2] \frac{1-[NO]^2}{1+k_i^+[NO]/(k_2^+[O_2]+k_3^+[OH])} K = \left(\frac{k_i^+}{k_i^-}\right)\left(\frac{k_2^+}{k_2^-}\right)
\]

where:

\[
K = \left(\frac{k_i^+}{k_i^-}\right)\left(\frac{k_2^+}{k_2^-}\right)
\]

In Equation (4.58), \([ ]\) denotes the concentration of species in \( mol/cm^3 \). The rate constants \( k_i \) are defined in Equation (4.57). The concentration of O is determined from the work of Westenberg[122] and the concentration of OH is determined from the correlation.
developed by Westbrook et al. The correlations for determining [O] and [OH] are given in Equations 4.60 and 4.61, respectively.

\[
[O] = 0.397T^{-0.5}[O_2]^{0.5}\exp\left(-31090 / T\right) \tag{4.60}
\]

\[
[OH] = 2.129 \times 10^{-4}T^{-0.5}[O]^{0.5}[H_2O]^{0.5}\exp\left(-4595 / T\right) \tag{4.61}
\]

The NO emission is updated in each calculation step according to the correlation given in Equation 4.58, where temperature \( T \) and concentration of \( O_2, N_2 \) are from the temperature model and gas composition model. NO emission is assumed to form only in the spray packet zone, while the unburned gas zone is not included for NO calculation. The NO emission is calculated in each packet and total NO emission is the summation of the NO in all packets.

**Model Validation**

The Quasi-D diesel combustion model is validated with experimental data given in the ignition delay section. Summary of test setup and tested cases are given in Table 4.2 and Table 4.3, respectively. A summary of parameters used to setup the simulation are given in Table 4.4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of iterations</td>
<td>[-]</td>
<td>500</td>
</tr>
<tr>
<td>Calculation step size</td>
<td>CA/cycle</td>
<td>0.558</td>
</tr>
<tr>
<td>Total number of packets</td>
<td>[-]</td>
<td>100</td>
</tr>
<tr>
<td>Number of packets in Y direction</td>
<td>[-]</td>
<td>20</td>
</tr>
</tbody>
</table>
Figure 4.15 shows the comparison between predicted and experimentally measured cylinder pressure and apparent heat release rate. Conditions correspond to low speed low load with 2 different EGR ratios. Fuel injection rate and duration are also included in the plots for reference. It is shown that the model accurately predicts the heat release rate and cylinder pressure for both 0% EGR and 20% EGR conditions. In the 0% EGR case, it can be observed that the two stages of combustion (premixed and mixing controlled) are well captured by the model. The premixed combustion contributes the initial spike of heat release and is followed by diffusion combustion with lower heat release rate. For the 20% EGR case, the combustion model captures the prolonged ignition delay due to the inclusion of EGR. Nevertheless, the peak rate of heat release does not increase due to the reduced oxygen concentration. This is enabled by the added chemical reaction rate limit discussed in Equation (4.38).
Figure 4.15. Validation of simulation with experimental data, low speed low load conditions. (A): without EGR; (B): with EGR.

Figure 4.16 shows the validation results at high speed, high load conditions with and without EGR. Again, predictions of both heat release rate and cylinder pressure profiles show good agreement with experimental data. The high-frequency fluctuations superimposed on the main trends is caused by the finite number of packets used in the model. The spray is divided into 100 packets to reach a balance between prediction accuracy and computational load. With increased packet number, the fluctuations of the heat release can be mitigated, but at the cost of increased computing time. It can be observed that the model accurately captured two stages of heat release in both EGR conditions. At high load conditions, the fraction of heat released from premixed combustion is much lower than that of low load conditions. This is due to the reduced ignition delay time and longer fuel injection duration, which releases more of the fuel
energy during the mixing controlled stage. The combustion model has sufficient fidelity to capture these details. When comparing the heat release profile between 0% EGR and 20% EGR cases, a longer ignition delay and lower peak premixed heat release rate are associated with the 20% EGR case. These two differences were captured by the combustion model due to the modified ignition delay correlation and added chemical reaction rate limit.
Figure 4.16. Validation of simulation with experiment data at high speed high load conditions. (a): without EGR; (b): with EGR.

The results shown in the above two figures are obtained from simulations without tuning the parameters, at different load, speed and EGR conditions. This displays good robustness of the model. The modified heat release model as well as the ignition delay correlation are key enablers of achieving this accuracy.

Figure 4.17 shows a comparison between simulation results from the model developed in this work and the model from Hiroyasu’s framework at the same operating condition. It is shown that the prediction result from the original Hiroyasu’s model displays a non-physical spike of heat release rate after start of combustion. On the contrary, the model developed in this work does a much better job in predicting the heat release history during the premixed combustion stage, thanks to the improved ignition delay and heat release sub-models.
Figure 4.17. Comparison between simulation results from the model developed in this work and the model from Hiroyasu’s framework.

Figure 4.18 shows the temperature prediction for different packets at low speed low load condition with no EGR. The $i_{pac}$ in the legend denotes the index of packet on the $x$ axis as defined in Figure 4.2. In this case the total number of packet sets on the $x$ axis (packets with same $x$ index) is 20. This figure shows the predicted temperature history in individual packets, where packets with smaller $i_{pac}$ are injected earlier than the packets with larger $i_{pac}$. This illustrates the fidelity of the model, i.e. its ability to capture the temperature distribution within the spray. This is in turn critical for estimating the emission formation. Together, models of the packet temperature and spray penetration provide spatial resolution of temperature within the spray. The prediction of local hot spots and temperature difference among different locations will have beneficial effect on the prediction of temperature-dependent emissions, especially NOx.
Figure 4.18. Simulated temperature history in individual packets.

Figure 4.19 shows the predicted temperature for burned, unburned and bulk gas temperature at both low speed low load, and high speed high load conditions. The EGR levels shown in this figure are 0% and 24% for low load condition and 0% and 25% for high load condition. Here the burned zone temperature is calculated as mass averaged temperature of all packets. For both cases, inclusion of EGR results in lower burned, unburned and bulk gas temperatures due to the higher heat capacity of products and altered combustion characteristics. The model is giving reasonable estimation results of temperature with or without EGR.
Figure 4.20 shows an example of the predicted heat transfer rates. The case shown in this figure is high speed high load condition without EGR. The heat loss from convective heat transfer, radiative heat transfer and total heat transfer are shown. The
figure also indicates the importance of including radiative heat transfer as it accounts for about 30% of total heat transfer rate at the peak of heat transfer rate and as high as 50% when approaching the end of the expansion stroke.

![Simulated heat transfer rate, high speed high load without EGR.](image)

Figure 4.20. Simulated heat transfer rate, high speed high load without EGR.

Figure 4.21 shows the prediction of NOx formation for both low load and high load conditions with or without EGR. The mass averaged packet temperature (burned zone temperature) is also included for reference. After NOx concentration reaches its peak, there is a short breakdown period where NOx concentration drops slightly and then settles as temperature drops and reactions freeze. The drop in NOx concentration during the breakdown period is small and hardly noticeable on the graph. It can be noticed that the NOx formation is very sensitive to temperature. In both low load and high load conditions, a slight change of temperature resulted in a much greater difference in NOx formation. Take the low load case for instance, the inclusion of 24% EGR resulted in a
200K drop of peak temperature, while the formation of NOx drops more than 70% compared to the condition with no EGR.

Figure 4.21. Simulated NOx formation history.
Figure 4.22 shows the comparison between predicted and experimentally measured engineout NOx emissions. The dashed lines are quadratic fit of data points. Clear trend is observed in both engine load conditions that NOx emissions drop quickly with increased EGR fraction. The model shows good agreement with experimental data in both low load and high load conditions. The NOx prediction capability is also an indication of good temperature estimation, given the sensitivity of NOx formation to the temperature.

Figure 4.22. Comparison between simulation predicted NOx concentration and experiment data.
In this work, a multi-zone diesel combustion model is developed and validated with experimental data. The model is based on the framework proposed by Hiroyasu et al. The new contributions enhance the capabilities of the model to make it suitable for studies of modern engines operating with high-injection pressures and significant EGR. In particular, (i) a new spray tip penetration sub-model is developed based on measurements obtained in a high-pressure, high-temperature constant volume combustion vessel, (ii) ignition delay correlation is modified to capture the effect of reduced oxygen concentration in engines with EGR, and (iii) an algorithm considering the chemical reaction rate of hydrocarbon-oxygen mixture improves prediction of the heat release rates.

The improved spray penetration model is developed with the help of experimental data from a constant volume chamber. The original spray tip penetration correlation developed by Hiroyasu et al. is modified to handle the higher injection pressure and smaller hole diameters of modern injectors. The density of the charge is included as an additional parameter, and model constants were tuned to arrive at good agreement with experiments over a range of representative conditions.

The ignition delay correlation and heat release model are modified to accommodate the inclusion of EGR. An improved predictive ignition delay correlation includes oxygen concentration as an added parameter to account for the effect of EGR. The new correlation is developed with the aid of experimental data from a single cylinder research engine with boosting and common rail injection. The modified ignition delay
correlation shows much better agreement with experimentally measured ignition delay at representative operation conditions with varying level of EGR.

Similarly to the motivation of developing a new ignition delay correlation, the existing heat release model is modified to account for the effect of EGR on the reaction rate of fuel. In the modified heat release sub-model, chemical reaction rate of the hydrocarbon oxygen mixture is included as an additional criterion. It limits the rate of heat of release at the beginning of premixed combustion, and captures the effect of reduced oxygen concentration on the chemical reaction rate when engine runs with EGR.

The combustion model is validated with experimental data at two different operation conditions with varying EGR levels. The model displays good agreement with experimental data in both heat release and cylinder pressures. The model also gives reasonable prediction of temperature in each packet, the unburned gas temperature and bulk cylinder temperature. The predicted engine out NOx emissions agrees very well with experiment over a range of EGR fractions, which is another indication that the model correctly estimates the in-cylinder gas temperature.

This work has provided a thorough description of the modeling scheme that can easily be used by other researchers. By varying the number of packets and calculation time step, a balance between computing power requirement and model fidelity can be reached based on the simulation goal. The model can help expedite the calibration or development process of a diesel engine, and can also be used for investigating new mixing-controlled combustion concepts.
CHAPTER FIVE
QUASI-D COMBUSTION MODELING OF DUAL-FUEL ENGINES

Introduction

Quasi-D modeling of dual-fuel combustion provides a very attractive compromise between model fidelity and computing efficiency. Challenges associated with this modeling approach are raised by the introduction of gaseous fuel into combustion chamber which greatly alters the combustion characteristics of conventional diesel engines. A dual-fuel engine involves features from both compression ignition and spark ignition engines. The fuel energy input includes in-cylinder direct injection of diesel and port fuel injection of NG. The combustion process includes auto ignition of diesel, multi-site ignition of NG by adjacent diesel flamelets, which is followed by simultaneous mixing-controlled combustion of diesel and flame propagation of NG. Since the two types of combustion happen simultaneously in a common space, it is inappropriate to model the combustion process from simply combining the existing modeling scheme for diesel and SI engines. To mention just a couple of obvious challenges, presence of NG in a surrounding fresh charge will affect diesel ignition delay and air entrainment into the spray; The existing SI flame propagation models assume a single ignition source and a spherical flame, while burning of NG in a dual-fuel engine starts at multiple sites, and leads to a flame engulfing the entire spray.

Quasi-D multi-zone models of dual-fuel combustion have been studied extensively in the published work [17, 18, 70, 87-92]. In the previous research efforts to develop a Quasi-D model for a dual-fuel engine, Papagiannakis et al.[70] proposed to
incorporate turbulent flame propagation modeling approach to represent the combustion of NG. The NG flame was assumed to propagate from the outer boundary of a diesel spray, which was approximated as a conical shape. However, the discussion of the combustion of diesel fuel was limited. Krishnan et al. [18] on the other hand, has incorporated detailed discussion of the diesel spray and combustion modeling, where a diesel spray was divided into multiple packets and treated individually. However, modeling of NG combustion is simplified. The author assumed NG flame fronts to propagate individually as spherical shape from each ignition site and does not interact with each other.

The approach proposed here combines and extends the two approaches described above. The diesel spray and combustion behavior is modeled by dividing injected diesel fuel into multiple packets, while the combustion of NG is modeled with the turbulent flame entrainment approach. The flame front is initiated from the outer boundary of the diesel spray, and the flame front propagates away from the spray until it hits the physical boundaries, i.e. either the wall or the adjacent conical flames. The two combustion models run in parallel to provide a complete prediction of the dual-fuel combustion process. Detailed information with regard to the evolving diesel spray, ignition, mixing controlled burning of diesel, and flame propagation of NG-air can be obtained from the model. Heat release histories of both fuels are traced separately, as well as the total.

The diesel combustion model developed here is based on the framework proposed by Hiroyasu et al. with several improvements of sub-models. The original sub-models integrated within the multi-zonal framework are intended to enhance predictiveness under
conditions relevant for dual-fuel operation. For the NG model, a new way of modeling the flame front area during NG flame propagation is proposed. The flame is assumed to initiate from the outer boundary of diesel spray and propagate into the space in the direction perpendicular to the diesel spray boundary, until it starts to interact with multiple geometric constraints. The algorithm incorporates geometrical information of all boundaries and provides a universal solution for various piston or cylinder head designs.

**Dual-fuel Combustion Modeling Scheme**

The modeling of diesel spray and combustion has been discussed in detail in the previous chapter. Figure 5.1 gives an illustration of dual-fuel combustion process. The depiction of diesel spray used here is from the work by Dec[25]. Burning of NG is added to the spray image by the author, to illustrate the conceptual model of dual-fuel combustion. Figure 5.1(1)-(6) gives a time-lapse description of the combustion process from SOI of diesel to the end of combustion, which is divided into 6 stages. Stage (1) shows the initial development of diesel spray right after the diesel fuel is injected into the NG-air mixture. After a short ignition delay period, diesel fuel auto-ignites and initiates the premixed combustion of diesel vapor and air mixture. In the meantime, the NG-air mixture surrounding the diesel spray is also ignited by the energy released from the combustion of diesel[66]. As the combustion progresses to stage (3), the combustion mode of diesel transfers from premixed burning to mixing controlled burning. Meanwhile, a NG flame front has formed surrounding the diesel spray and then propagate into the unburned NG-air mixture. At stage (4), as the injection event continues, diesel
fuel keeps burning in the mixing-controlled mode and soot continues to form in the fuel-rich zone, while NG flame propagates into the end gas zone. Due to the heat released from diesel and NG combustion, the NG-air mixture in the end gas zone is subject to high pressure and temperature, thus there is a chance for an auto-ignition (knock) to take place[5], especially at higher loads. At stage (5), diesel continues to burn in a mixing controlled mode until all diesel fuel is consumed. Most of the soot accumulated in the spray head vortex oxidizes, and the remaining mass eventually leaves the cylinder with exhaust gases. The relative length of the combustion depends on the substitution rate, i.e. the mass of diesel fuel for a given load point. As NG flame propagates into the end gas zone, the flame fronts formed from each individual spray interact with neighboring ones and merges as a unit flame front. As combustion progress towards the end, as shown in stage (6), diesel fuel is all consumed and fraction of the remaining soot is oxidized by the burning of the lean NG charge. The flame propagation of NG terminates as the flame front reaches the wall. Due to the lower laminar flame speed of lean NG-air mixture, there is a chance that a small portion of NG in the end gas zone remains unburned at exhaust valve opening (EVO), especially at low load conditions.

The Quasi-D combustion model developed in this dissertation has the fidelity of generating spatial resolution of temperature in the spray. This is enabled by dividing the spray into multiple packets and track them individually, and the capability of estimating temperature in each individual packet is demonstrated in Figure 4.18. However, the location where knock occurs, i.e. whether it occurs in between the sprays or at the end
gas zone next to the wall, cannot be predicted from the model, due to the single-zone unburned gas assumption.

Figure 5.1 A time-lapse illustration of dual-fuel combustion process, developed around original illustrations of spray development proposed by Dec [25].

Figure 5.2 gives a flow chart of the simulation process. In each engine cycle, the calculation scheme shown in Figure 5.2 is iterated multiple times to obtain crank angle resolved in-cylinder states. The engine cycle simulation starts at IVC and ends at EVO,
thus no mass transfer occurs between ambient and in-cylinder charge during the simulation span. The initial in-cylinder gas composition is either premixed NG-air or NG-air-EGR mixture. In the compression stroke before SOI, the thermodynamics model calculates the in-cylinder temperature and pressure with consideration of heat loss to the wall. The temperature and pressure obtained in this process is used to estimate the ignition delay. After SOI, liquid diesel is injected into the cylinder and it triggers the sub-models for calculating spray tip penetration, air-NG entrainment and fuel droplets evaporation. The spray tip penetration model estimates the penetration length of each packet, which serves as the input for the latter air-NG entrainment and fuel evaporation calculations. The spray tip penetration calculation is followed by air-NG entrainment and fuel evaporation calculations. The air entrainment model estimates the rate of air-NG mixture entraining into each packet while fuel evaporation model outputs the evaporation rate of diesel droplets and diesel vapor mass in each packet. In this work, NG is allowed to entrain into the packets before SOC. The NG entrainment is terminated after SOC since the burning mode of NG is transformed into turbulent flame propagation. The outputs of these air-NG entrainment and fuel evaporation sub-models provide information for calculating the heat release rate in each packet.

After the ignition delay period, the combustion starts and it triggers sub-models for calculating heat release from diesel in each packet and NG. The NG entrained into the packets during the ignition delay period is consumed quickly after SOC and NG entrainment is terminated after that point. In each packet, three possible scenarios are considered in the heat release model: air entrainment controlled, fuel evaporation
controlled and reaction rate controlled, where heat release rate is either determined by available fuel vapor or air mass in the packet or limited by the chemical reaction rates. As the heat released from diesel fuel ignites its surrounding NG-air mixture, the combustion of NG is self-sustaining and the flame propagates into the end gas zone similar to that in a spark ignited engine. The total heat release of dual-fuel combustion is the sum of contributions from both fuels. In parallel to the above mentioned models, the thermodynamics model runs in each calculation step to update gas composition and thermodynamic properties in each packet as well as the rest of cylinder charge. The above mentioned sub-models will be discussed in detail in latter sections.

Figure 5.2 A schematic description of computing process in the dual-fuel combustion model
Modeling of Diesel Spray and Combustion

Air-NG Entrainment Model

The rate of air entrained into each packet is calculated according to the correlation developed by Hiroyasu and Arai[106], as given in Equation(5.1). Air entrainment rate is determined by the mass of fuel in the packet $m_{f0}$, injection velocity $v_0$, fuel and air density $\rho_f, \rho_a$, break up time coefficient $\alpha$, radial weighting function $E_x$, nozzle hole diameter $d_0$ and mass of air entrained into the packet $m_a$. The ODE is updated in every calculation step to output mass of air entrained into the packet. The injection velocity $v_0$ is obtained as given in Equation(5.2), which is derived from the spray tip penetration model.

\[
\frac{dm_a}{dt} = \frac{2m_{f0}^2v_0^2}{\sqrt{v_0} \left( \frac{\rho_f}{\rho_a} \right)^{1/4} \sqrt{\alpha E_x d_0 (m_a + m_{f0})}}
\]  \hspace{1cm} (5.1)

\[
v_0 = 0.70 \left( \frac{\rho_a}{\rho_i} \right)^{-0.25} \sqrt{\frac{2\Delta P}{\rho_i}}
\]  \hspace{1cm} (5.2)

At diesel only conditions, only air and EGR are entrained into the spray, while at dual-fuel conditions, the entrained mass also includes NG. Entrained NG mass can be derived from the mass fraction of NG in the premixed NG-air mixture at IVC $x_{NG}$, as given in Equation(5.3), where $\dot{m}_{NG}$ is the NG entrainment rate into the packet. The mass entrainment rate into the diesel spray is zero after SOC.
Heat Release Model

It is assumed that in each packet only diesel vapor and NG react with surrounding air, while fuel droplets in liquid state are not involved in combustion. The mass of fuel burned, including both diesel and NG in a packet in each calculation step is determined by the mass of diesel vapor, NG and air and chemical reaction rates of both fuels.

Equations (5.4) and (5.5) give the scheme to determine the mass of fuel burned in each calculation step, where $\phi$ is the total equivalence ratio in the packet where both fuels are included; $AFR_{stoich}$ is the stoichiometric air fuel ratio and is obtained from $m_a$, $m_{fg}$ and $m_{NG}$, which are the mass of air, diesel vapor and NG in the packet, respectively; $\dot{m}_{chemD}$ and $\dot{m}_{chemNG}$ are chemical reaction rates of diesel-air and NG-air mixtures, respectively; $\Delta m_D$ and $\Delta m_{NG}$ are the mass of diesel and NG burned in a packet in each calculation step.

$$\Delta m_D = \begin{cases} m_a m_{fg} / (m_{fg} + m_{NG}) / AFR_{stoich} & \phi > 1 \\ m_{fg} & \phi < 1 \\ \dot{m}_{chemD} \Delta t & \Delta m_D > \Delta m_{chemD} \end{cases}$$ (5.4)

$$\Delta m_{NG} = \begin{cases} m_{NG} m_{NG} / (m_D + m_{NG}) / AFR_{stoich} & \phi > 1 \\ m_{NG} & \phi < 1 \\ \dot{m}_{chemNG} \Delta t & \Delta m_{NG} > \Delta m_{chemNG} \end{cases}$$ (5.5)

When the fuel/air mixture is richer than stoichiometry ($\phi > 1$), fuel mass burned $\Delta m_D$ and $\Delta m_{NG}$ are determined by the available air mass, $AFR_{stoich}$ and the weighting
between the mass of diesel vapor and NG. On the other hand, when the fuel/air mixture is leaner than stoichiometry, $\Delta m_D$ and $\Delta m_{NG}$ is determined by the mass of fuel vapor $m_{fg}$ and mass of NG $m_{NG}$ in the packet, respectively. When the mass of fuel burned at each calculation step determined from the first two criteria is smaller than the chemical reaction rate limit $\dot{m}_{chemD}$ or $\dot{m}_{chemNG}$, the burn rate is determined from the result of the first two criteria. On the contrary, when the mass fuel burned is greater than chemical reaction rate limit, the burn rate is then determined by the result of the third criterion. The chemical reaction rates of diesel-oxygen and NG-oxygen mixtures can be determined from the following formulas[79]:

$$
\dot{m}_{chemD} = A_d \exp \left( \frac{-E_a}{RT} \right) \left[ C_{12}H_{26} \right]^{0.25} \left[ O_2 \right]^{1.5} V_{pac} \cdot M_D
$$

$$
\dot{m}_{chemNG} = A_{NG} \exp \left( \frac{-E_a}{RT} \right) \left[ CH_4 \right]^{-0.3} \left[ O_2 \right]^{1.3} V_{pac} \cdot M_{NG}
$$

(5.6)

where $C_{12}H_{26}$ is used to approximate the chemical composition of diesel ($n$-dodecane) and $CH_4$ is used to approximate NG, $\dot{m}_{chemD}$ and $\dot{m}_{chemNG}$ are the chemical reaction rates of diesel and NG in g/s, respectively; $A_d$ and $A_{NG}$ are adjustable constants for diesel and NG, which are assumed as $2.5 \times 10^{10}$ and $8.3 \times 10^5$, respectively; $E_a$ is activation energy with constant value of 30kcal/mol, $R$ is universal gas constant in 0.001987kcal/mol/K, $T$ is gas temperature in the packet in K, $V_{pac}$ is packet volume in cm$^3$, $M_D$ and $M_{NG}$ are the molecular weights of diesel and NG in g/mol and $[C_{12}H_{26}]$, $[CH_4]$, $[O_2]$ denote the concentration of diesel vapor, NG and oxygen in mol/cm$^3$.

With the aforementioned method to determine mass of fuel burned in each calculation step, the total heat release rate from the combustion of fuel $\dot{Q}_{fuel}$ is given in
Equation (5.7), where $LHV_D$ and $LHV_{NG}$ are the lower heating values of diesel and NG and $n_{pac}$ is the total number of packets.

$$\dot{Q}_{fuel} = \sum_{j=1}^{n_{pac}} \left( \frac{LHV_{NG} \cdot \Delta m_{NG} + LHV_D \cdot \Delta m_D}{\Delta t} \right)$$

(5.7)

Modeling of NG Combustion

As have been shown in Figure 5.1, the combustion of NG is initiated from the burning of premixed diesel-air mixture. The rest of NG-air mixture is then consumed in the form of turbulent flame propagation. In this work, the burning of NG is divided into two stages: The first stage is the combustion of NG entrained into the diesel spray before SOC as have been discussed in the previous section, while the second stage is the self-sustaining combustion of NG-air mixture in the form of turbulent flame propagation.

The flame propagation of NG-air mixture is assumed to initiate from the outer boundary of the diesel sprays. As shown in Figure 5.3, the flame front propagates into space in the direction perpendicular to the outer boundary of a diesel spray\[70\]. Since the NG-air mixture is ignited by the combustion of diesel, the characteristics of this spray outer boundary is determined at SOC. For the simplicity of numerical calculation, the outer boundary of a diesel spray is approximated as a conical shape with a hemisphere attached to the bottom of the cone. Once flame propagation is initiated, the flame front is assumed to propagate with the same speed in all directions until being cut off by other constrains such as cylinder wall, piston or the flame fronts initiated from surrounding sprays.
Turbulent Flame Propagation Model

The combustion of NG is modeled based on the turbulent flame propagation widely used in 0-D, 1-D simulations of SI engines. It is a Quasi-D modeling approach, where the in-cylinder space is separated into two zones: burned and unburned zone, and geometric interaction of the flame front with physical boundaries are fully resolved. In the context of a dual-fuel engine, a simple two-zone assumption is not sufficient since two fuels are burning in two different modes simultaneously. In this work, a multi-zone diesel spray-combustion model is running in parallel with the NG turbulent flame propagation model; thus an original definition of zones and boundaries is needed. Since the combustion of NG happens after SOC of diesel, part of the in-cylinder charge has already entrained into the diesel spray and is not included in the modeling of NG flame propagation. After the ignition of NG, it is assumed that only unburned NG-air mixture is entrained into the burning zone, while all the diesel vapor and burned products from the
combustion of diesel are retained in the packets and are not participating the NG flame propagation.

According to the turbulent flame entrainment modeling approach proposed by Tabaczynski et al.[124], the rate of mass entrained into the reaction zone is represented as:

$$\frac{dm_e}{dt} = \rho_u A_f (S_L + u')$$  \hspace{1cm} (5.8)

where $m_e$ is the mass entrained into the reaction zone, $\rho_u$ is unburned gas density, $A_f$ is the surface area of flame front, $S_L$ is laminar flame speed and $u'$ is turbulent intensity. The calculation of $A_f$, $S_L$ and $u'$ will be discussed in detail in latter sections. Once unburned gas is entrained into the reaction zone, the NG-air mixture burns with a rate proportional to the unburned mass in the entrainment front. The rate of mass burned can be obtained as:

$$\frac{dm_b}{dt} = \frac{m_e - m_b}{\tau}$$  \hspace{1cm} (5.9)

where $m_b$ is the burned mass and $\tau$ is the characteristic burning time. The characteristic burning time is defined as the time it takes to travel the distance of Taylor microscale $\lambda$ with laminar flame speed $S_L$ [124]:

$$\tau = \frac{\lambda}{S_L}$$  \hspace{1cm} (5.10)

The laminar flame speed of NG-air mixture $S_L$ can be obtained as[33]:
\[ S_L = S_{L0} \left( \frac{T_u}{T_0} \right)^{\alpha} \left( \frac{P}{P_0} \right)^{\beta} \left( 1 - 2.06\bar{x}_b^{0.77} \right) \] (5.11)

where \( S_{L0}, \alpha, \beta \) are constants for a given fuel and equivalence ratio, \( T_0 = 298K \) and \( p_0 = 1atm \) are reference temperature and pressure, \( T_u \) is unburned gas temperature, \( p \) is cylinder pressure and \( \bar{x}_b \) is the mole fraction of burned gas diluent. The three constants \( S_{L0}, \alpha \) and \( \beta \) for NG are defined as given in Equations (5.12) and (5.13) [125], where \( B_m = 0.49m/s, B_\phi = -0.59m/s, \phi_m = 1.39 \) and \( \phi \) is equivalence ratio.

\[ S_{L0} = B_m + B_\phi \left( \phi - \phi_m \right)^2 \] (5.12)

\[ \alpha = 0.68\phi^2 - 1.7 + 3.18 \]
\[ \beta = -0.52\phi^2 + 1.18\phi - 1.08 \] (5.13)

The Taylor Microscale \( \lambda \) used in Equation(5.10) is the spacing of turbulent vortex tubes by its physical definition[124]. It can be represented as a function of integral length scale \( L \) and turbulence intensity \( u' \):

\[ \frac{\lambda}{L} = \left( \frac{15}{A} \right)^{0.5} \left( \frac{u'L}{\nu} \right)^{-0.5} \] (5.14)

where \( A = 1 \) for perfect isotropy and \( \nu \) is kinematic viscosity. The kinematic viscosity of unburned gas can be obtained from the correlation given in Equation(5.15), where \( T_u \) and \( \rho_u \) are unburned gas temperature and density.

\[ \nu = 3.3 \times 10^{-7} \frac{T_u^{0.7}}{\rho_u} \] (5.15)
Before SOC, the integral length scale $L$ used in Equation (5.14) can be represented as a function of cylinder volume $V$ and bore size $B$, as given in Equation (5.16). The calculation of integral length scale after combustion will be discussed in the latter section.

$$ L = \frac{4V}{\pi B^2} \quad (5.16) $$

The turbulence intensity $u'$ before SOC is determined from the turbulent energy cascade model, also known as the $k - \varepsilon$ model[126]. In this model, mean kinetic energy $K$ is converted to kinetic turbulent energy $k$, and kinetic turbulent energy is then converted to heat via viscous dissipation. The mean kinetic energy and kinetic turbulent energy are defined as given in Equations (5.17) and (5.18), where $m$ is the mass in the cylinder and $U$ is mean flow velocity.

$$ K = \frac{1}{2} m U^2 \quad (5.17) $$

$$ k = \frac{3}{2} m u'^2 \quad (5.18) $$

The change rate of mean kinetic energy and kinetic turbulent energy $\dot{K}, \dot{k}$ are given as:

$$ \frac{dK}{dt} = \frac{1}{2} \dot{m}_i v_i^2 - P_t - K \frac{\dot{m}_i}{m} \quad (5.19) $$

$$ \frac{dk}{dt} = P_t - m \varepsilon - k \frac{\dot{m}_i}{m} \quad (5.20) $$

where $\dot{m}_i$ and $\dot{m}_e$ are the mass flow rate into and out of the cylinder, $v_i$ is velocity of flow into the cylinder, $P_t$ and $\varepsilon$ are the production and dissipation rate of turbulent kinetic energy, respectively. Since the cycle simulation starts at IVC and end at EVO, no mass
transfer exists between cylinder and ambient during the simulation span, thus the terms with valve mass flow rates $\dot{m}_i$ and $\dot{m}_e$ are zero. The production and dissipation term for turbulent kinetic energy $P_t$, $\varepsilon$ are defined as given in Equations (5.21) and (5.22), where $c_\beta$ is an adjustable constant.

$$P_t = 0.3307 c_\beta \left( \frac{K}{L} \right) \left( \frac{k}{m} \right)^{0.5}$$  \hspace{1cm} (5.21)

$$\varepsilon = \frac{u'^3}{L} = \left( \frac{2k}{3m} \right)^{1.5}$$  \hspace{1cm} (5.22)

During the combustion, the turbulence intensity and integral length scale are governed by the conservation of angular momentum of large eddies[124]:

$$\frac{L}{L_0} = \left( \frac{\rho_{u0}}{\rho_u} \right)^{1/3} \quad \frac{u'}{u'_0} = \left( \frac{\rho_u}{\rho_{u0}} \right)^{1/3}$$  \hspace{1cm} (5.23)

where $L_0$, $u'_0$ and $\rho_{u0}$ are integral length scale, turbulence intensity and unburned gas density at SOC.

**Development of a Flame Geometry Model for Dual-fuel Combustion**

The flame front area $A_f$ appeared in Equation(5.8) is defined as the surface area of the leading edge of flame. It requires a new model to capture geometric features of the flame growing from multiple ignition sites and eventually surrounding the entire spray.

Flame front area governs the mass entrainment rate into the reaction zone thus this parameter must be addressed carefully. In conventional SI engines, it is generally accepted that the flame front initiates from the location of spark and propagates into the
space with a spherical shape. In the context of dual-fuel engines, the ignition of a diesel spray generates multiple ignition sites for the surrounding NG-air mixture. Those ignition sites then form a unit flame front which travels in the direction perpendicular to the outer boundary of diesel spray. Under this circumstance, the flame front can no longer be considered as a spherical shape. Instead, an original flame front model which has the fidelity to predict the surface area of the flame surrounding the spray and its interaction with constraints is needed.

In this work, a new flame geometry model is developed to predict the flame front area of NG-air flame in a dual-fuel engine. A detailed model is proposed to track the evolution of flame front initiated from each diesel spray. The in-cylinder space is divided into a number of slices equals to the number of diesel injector holes. It is assumed that diesel sprays injected from each injector hole are identical and uniformity is assumed among all slices, thus the flame geometry model only need to be applied to one slice while rest of slices have the identical results. The NG flame is assumed to evolve from multiple ignition sites, where individual flamelets propagate and merge into a flame front that engulfs the diesel spray. The fully-formed front subsequently propagates outwards until it eventually starts to interact with boundaries and reaches the furthest point on the periphery.

Initial Conditions

The NG flame front is assumed to originate from the outer boundary of a diesel spray, thus the geometry of diesel spray at SOC determines the initial conditions of NG
combustion. Figure 5.4 shows geometrical definition of a diesel spray at SOC. The shape of the diesel spray is approximated by a combination of a cone and a hemisphere, which agrees well with optical studies of diesel sprays[25]. The 2-D view is from the side of the cylinder, where the top dotted line represent the surface of cylinder head.

![Figure 5.4 Geometrical definitions of a diesel spray at SOC](image)

The spray tip penetration at SOC is represented as $L_{p0}$, which can be obtained from the spray penetration model given in Equations (4.9) and (4.13). The spray angle $\theta$ is obtained from the correlation developed by Hiroyasu and Arai[106]:

$$2\theta = 0.05 \left( \frac{\rho_a \Delta P d_0^2}{\mu_a^2} \right)^{1/4}$$

(5.24)

where $\rho_a$, $\mu_a$ are density and dynamic viscosity of in-cylinder gas at SOI, $\Delta P$ is the pressure difference between the injector and ambient gas and $d_0$ is the injector hole diameter. The angle between the spray centerline and cylinder head is represented as $\alpha$.

At this initial condition, the height of the cone $x_0$ and the diameter of the hemisphere $r_0$ can be obtained as:
Free Evolving Flame Front

As the flame front forms from the outer boundary of diesel spray, it propagates freely into the space in the direction perpendicular to the diesel spray outer boundary. Assuming there is no constrains to the propagation of flame front, the geometry of flame front is represented in Figure 5.5.

For this free evolving flame front, it is assumed that the speed of flame propagation is identical at every location, which applies to both the cone and hemisphere. At any moment of flame propagation, the distance between the injector hole and the furthest location of flame front relative to injector $L_p$ is defined as:

$$x_0 = \frac{L_{p0}}{1 + \tan \theta} \quad r_0 = x_0 \tan \theta$$

(5.25)
\[ L_p = L_{p0} + \int (u' + S_L) dt \]  

(5.26)

where \( L_{p0} \) is obtained from initial conditions and \( \int (u' + S_L) dt \) is the distance of flame front traveled after SOC. At any moment, this distance traveled is identical at every location of the flame front. With \( L_p \) known, the radius of the hemisphere flame front \( r \) is defined as the difference between \( L_p \) and initial height of the cone \( x_0 \):

\[ r = L_p - x_0 \]  

(5.27)

The furthest distance between flame front and the injector hole in the direction perpendicular and parallel to the cylinder head \( X_p \) and \( Y_p \) are defined as given in Equation (5.28).

\[ X_p = x_0 \cos \alpha + r \quad Y_p = x_0 \sin \alpha + r \]  

(5.28)

Interaction with Boundaries

In real-world engine conditions, the NG-air flame initiated from the diesel spray will not always propagate freely into the space. Instead, the flame front eventually interacts with surrounding boundaries, including cylinder head, cylinder wall, piston and other flame fronts from surrounding sprays. In that case, parts of the flame front are cut-off by the wall/boundary, and the active flame front area is reduced. All these constrains need to be taken into consideration for the calculation of flame front surface area in each computing step.

To realize this, geometrical information of the cylinder, especially the piston geometry is needed. Figure 5.6(a) shows the shape of the piston used in the experiments.
The piston is bowl-in-piston type, which is commonly used in diesel and dual-fuel engines. A detailed modeling of the geometry of this piston top in a Quasi-D model would require a detailed mesh, and the model would become bulky and computationally intensive. In addition, a detailed drawing would be required from a manufacturer and that is typically considered to be proprietary information. Instead of modeling the piston top in full detail, its geometry can be approximated to as shown in Figure 5.6(b), where the piston bowl is further approximated to two boundaries parallel to cylinder head and wall, respectively, which are depicted as dashed lines. This approximation is for the convenience of solving the geometrical interactions between the flame front and piston bowl.

Figure 5.6 (a) Geometry of the piston from the engine used in this work; (b) Approximation of the piston geometry on a 2-D plane.

To solve the interaction between flame front and cylinder head, wall and piston top, the cylinder space is divided into 9 identical slices as shown in Figure 5.7 (for a 9-
hole injector). The geometries defined in Figure 5.7 sets the basic framework for the flame geometry model. Each slice of in-cylinder space is approximated with a triangular prism, where O1-O2-O3 defines plane B, which represents the cylinder head; O1-O4-O10-O9 defines plane A, which is a vertical slice that is coplanar to the spray centerline; O5-O6-O8-O7 defines plane C, which is a slice perpendicular to the spray centerline. The shaded area on plane C is the projection of the enflamed area, where the outer boundary of the shaded area is the projection of flame front. The numerical scheme to arrive at the total flame front surface area is to calculate the projection of flame front on plane C at every possible location and integrate them along the spray centerline. O5-O6-O8-O7 is the constraint for the flame front projection on plane C, where O5-O6 defines cylinder head, O11-O12 defines piston top, and O5-O7, O6-O8 defines the surrounding slices. When the projected flame front on plane C are within the constrains, the flame front is not touching any of the constraining boundaries. On the other hand, when the projected flame front intersects with any of the constrains, the part that is outside of the boundaries is ‘cut-off” and is not included in the calculation of total flame front area. The location of plane C and the shape of shaded area shown in this figure is a typical example to illustrate the cycle calculations. During the solving process, the position of piston changes all the time and plane C need to be taken at every possible locations. The geometrical definitions given in this figure apply for all conditions and remain consistent in the latter sections.
The Plane A defined in Figure 5.7 can be further illustrated in Figure 5.8. Here a reference plane is defined as a plane perpendicular to the spray centerline and is coplanar to the injector. The distance between the reference plane and Plane C is defined as $x$ and the radius of projected free evolving flame front is defined as $r_x$. The distance between the piston top and cylinder head is defined as $h_{p2}$. As have been shown in Figure 5.6, the
piston bowl is approximated to a cylindrical shape for the continence of numerical calculations. The distance between piston top and the approximated plane of piston bowl is defined as \( h_{p0} \), while the distance between cylinder head and piston bowl plane is \( h_{p1} \).

Figure 5.8 Further illustration of geometrical framework in a 2-D plane.

The radius of projected free evolving flame front \( r_x \) can be obtained as defined in Equation (5.29). Three scenarios are considered based on the distance between reference plane and Plane C \( x \). When \( x \) is lesser than \( x_0 \), it is assumed that the flame front travels in the direction in parallel to the reference plane. Since the flame front has the same traveling speed at any location, the distance of flame front traveled in this scenario is the same as the location where the flame evolves as a hemisphere, which is \( r - r_0 \) at any
moment. When $x$ is greater than $x_0$ and lesser than the furthest location of flame front relative to the reference plane, $r_x$ is obtained as the radius of the slice of the hemisphere. When $x$ is greater than $x_0 + r$, $r_x$ is zero.

$$r_x = \begin{cases} 
  x \tan \theta + r - r_0; & 0 < x \leq x_0 \\
  \sqrt{r^2 - (x - x_0)^2}; & x_0 < x \leq x_0 + r \\
  0; & x > x_0 + r
\end{cases}$$  \hspace{1cm} (5.29)

The distance between piston top and cylinder head $h_{p2}$ and the distance between the piston bowl plane and cylinder head $h_{p1}$ can be obtained according to Equation (5.30), where $V_{cyl}$ is the instant volume of the cylinder and $R_{cyl}$ is the radius of the cylinder which equals to Bore/2. In this work, cylinder volume is calculated by assuming the piston top is flat, thus the piston bowl volume is neglected when obtaining $h_{p2}$.

$$h_{p2} = \frac{V_{cyl}}{\pi R_{cyl}^2} \quad h_{p1} = h_{p2} + h_{p0}$$ \hspace{1cm} (5.30)

Figure 5.9 defines a coordinate system for plane A. In this two-dimensional coordinate system, the X axis is coplanar to the cylinder head while the Y axis is coaxial to the centerline of the cylinder. The cross point of X and Y axes is defined as the origin. The Plane C is extended on both directions to intersect with every possible planes. The intersection lines in the 3-D space are reduced to points A, B, C, D, E and O in this 2-D plane, where point A stays on line $Y = -h_{p1}$, point B stays on line $Y = -h_{p2}$, point C stays on line $Y = 0$, point D stays on line $X = R_{cyl}$ and point O is the intersection point between line DE and the spray centerline. The geometrical positions of these points enable a universal numerical solution of the flame front area.
With the coordinate system defined, the functions of constraints and coordinates of intersection points can be easily obtained. The function of the line representing Plane C, which is line DE, can be defined as:
\[ Y = \frac{1}{\tan \alpha} X - \frac{x}{\sin \alpha} \]  

(5.31)

With the function of line DE, the coordinates of points A, B, C, D, E and O can be obtained by solving the combined equations of line DE and other constraining lines:

A: \[
\left[ \tan \alpha \left( \frac{x}{\sin \alpha} - h_{p1} \right), -h_{p1} \right]
\]

B: \[
\left[ \tan \alpha \left( \frac{x}{\sin \alpha} - h_{p2} \right), -h_{p2} \right]
\]

C: \[
\left[ \frac{x}{\cos \alpha}, 0 \right]
\]

D: \[
\left[ R_{cyl}, \frac{R_{cyl}}{\tan \alpha} - \frac{x}{\sin \alpha} \right]
\]

E: \[
\left[ 0, -\frac{x}{\sin \alpha} \right]
\]

O: \[
\left[ x \cos \alpha, -x \sin \alpha \right]
\]

In this case, the piston bowl is approximated to a flat surface with a function of \( Y = -h_{p1} \) for the convenience of numerical calculation. In this coordinate system, the piston bowl or even the cylinder head can be further defined as any functions that represents the true shape. The coordinates A-E and O can still be easily obtained by solving the combined equation of Plane C and the constraining surfaces.

To obtain the solution of total flame front area, Plane C need to be taken at every possible locations. In the coordinate system defined above, Plane C is allowed to move between \( x = 0 \) and \( x = x_t \). The furthest location \( x_t \) is defined as:

\[ x_t = \left( h_{p2} \tan \alpha + R_{cyl} \right) \cos \alpha \]  

(5.32)
Now the geometries in Plane A have been fully defined. Figure 5.10 gives the geometrical definition of Plane C. As have been shown in Figure 5.7, each slice of the cylinder volume is assumed as a triangular prism, thus the intersection plane between plane C and the cylinder volume slice always results in a triangle, shown as the dashed outline in Figure 5.10, where the lowest point corresponds to the point E shown in Figure 5.9. The top line of the triangle corresponds to the cylinder head and the rest two lines are representing the boundary between the slice and neighboring slices. The dashed circle defines the projection of flame front on this plane, while the solid lines shown in this figure which has a trapezoidal shape are representing the constraints of the flame front. When the projection of flame front is beyond the trapezoidal constraints, it is considered to be cut-off by the constraints. In Plane C, the projected flame front that is within the constraints is defined as the effective flame front, while the total length of the effective flame front is defined as the effective flame length.
With the geometrical definition shown in Figure 5.10, the geometrical information of the trapezoidal constraints can be easily obtained. Here two reference lines are defined which both intersect with the center of projected flame front where one is parallel and another is perpendicular to the cylinder head. The distances between the two horizontal lines and the horizontal reference are defined as $l_1$ and $l_2$. The two lengths which further defines the position of trapezoidal constraints in relative to the vertical references are $h_1$ and $h_2$, respectively. The numerical representation of $l_1$ can be summarized as:
where $|CO|$ and $|DO|$ are the length of line CO and DO defined in Plane A, which can be obtained from the coordinates of each points given above. $Y_C$, $Y_D$ and $Y_O$ are the Y coordinates of points C, D and O. Similarly, $l_2$ can also be summarized as:

\[

l_2 = \begin{cases} 
|OE|; & X_A \leq 0 \\
|OB|; & X_B \geq r_\theta \wedge Y_O \geq Y_B \\
-|OB|; & X_B \geq r_\theta \wedge Y_O < Y_B \\
|OA|; & X_A > 0 \wedge X_B < r_\theta \wedge Y_O \geq Y_A \\
-|OA|; & X_A > 0 \wedge X_B < r_\theta \wedge Y_O < Y_A 
\end{cases} \quad (5.34)
\]

where $X_i$ represents the X coordinates of each points defined in Plane A. In the above definition of $l_1$ and $l_2$, when the number becomes negative, it means the location of the constraints are on the opposite side of the reference line shown in Figure 5.10. The height of the triangular boundary, which is defined as $s_1$ in Figure 5.10, can be obtained as:

\[
s_1 = \frac{x}{\sin \alpha \cos \alpha} \quad (5.35)
\]

Similarly, the distance between the cylinder head and the lateral reference line $s_2$ can be represented as:

\[
s_2 = x \tan \alpha \quad (5.36)
\]

The angle which determines the shape of the triangular boundary, define as $\alpha_{c_1}$ in Figure 5.10, can be obtained as:
\[ \alpha_{c1} = \arctan \left( \sin \alpha \tan \beta \right) \]  

(5.37)

where \( \beta \) is the same as defined in Figure 5.7, which is determined by the number of injector holes. With above defined parameters, the position of trapezoidal constraints relative to the vertical references are \( h_1 \) and \( h_2 \) can be obtained as:

\[ h_1 = (l_1 + s_1 - s_2) \tan \alpha_{c1} \quad h_2 = (s_1 - s_2 - l_2) \tan \alpha_{c1} \]  

(5.38)

Solving the Flame Front Area

As mentioned in the last section, the total length of the effective flame front in Plane C is defined as the effective flame length. This section gives the numerical solution of this effective flame length. Once this length is found in each Plane C, it can be integrated along the spray centerline to arrive the total flame surface area. For ease of numerical calculation, the right half of Figure 5.10 is tilted counterclockwise for 90° and is represented as shown in Figure 5.11, where the effective flame length is represented as \( l_x \). Since the geometry shown in Figure 5.10 is symmetrical with respect to the vertical reference line, the total effective flame length in this 2-D plane is \( 2l_x \).
In the geometry defined in Figure 5.11, when the projected flame front is beneath the constraints, the length of this flame front is considered as effective flame length and vise versa. To arrive a universal numerical solution, another coordinate system is defined. In this figure, a 2-D coordinate system is defined where X and Y axes are marked. To arrive a solution of effective flame length $l_x$, the relative geometrical position of projected flame front and constraints are evaluated alone the X axis from $X = -r_x$ to $X = r_x$. At each point on both the projected flame front and constraints which satisfies $X = x_c$, the Y coordinates are defined as $Y = y_c$ and $Y = y_l$. By evaluating $y_c$ and $y_l$ at each $x_c$, the total length of $l_x$ can be obtained by discrete integration.

When $X = x_c$ is satisfied, $y_l$ can be determined by the geometry of the constraints. Here the Y coordinates of constraints when $x_c < -l_1$ or $x_c > l_2$ are set to
zero to ensure the effective flame length is always zero at these conditions. The
numerical solution of $y_l$ is given as:

$$ y_l = \begin{cases} 0; & x_c \leq -l_1 \\ -\frac{(x_c - l_2)(h_1 - h_2)}{l_1 + l_2} + h_2; & -l_1 < x_c \leq l_2 \\ 0; & x_c > l_2 \end{cases} \quad (5.39) $$

Similarly, $y_c$ can be determined using the geometry of the projected flame front.

The numerical solution of $y_c$ is given as:

$$ y_c = \begin{cases} 0; & x_c \leq -r_x \\ \sqrt{r_x^2 - x_c^2}; & -r_x < x_c \leq r_x \\ 0; & x_c > r_x \end{cases} \quad (5.40) $$

With the information of $y_l$ and $y_c$, the discrete segment of effective flame length
$dl_x$ can be obtained by evaluating the geometrical relationship between projected flame
front and constraints at each location. The $dl_x$ can be represented as a function of the
coordinate of the X axis $dl_x = f(x_c)$. By integrating $dl_x$ alone the X axis, the total
effective flame length $l_x$ can be obtained as:

$$ l_x = \int_{-r_x}^{r_x} f(x_c)dx_c \quad (5.41) $$

The discrete segment of effective flame length $dl_x = f(x_c)$ can be determined
from the geometrical information of the projected flame front and the relative relation
between $y_l$ and $y_c$. When $y_c$ is greater than $y_l$, the projected flame surface is outside the
constraints, which indicates the flame is being ‘cut-off’ by constraints at this location,
thus $dl_x$ is 0. In contrast, when the projected flame front is within the constraints, the
effective flame length can be obtained by solving alone the projected flame front. The numerical solution of $f(x_c)$ is summarized as:

$$f(x_c) = \begin{cases} \frac{2r_x}{\sqrt{r_x^2 - x_c^2}}; & y_c \geq y_x \\ 0; & y_c < y_x \end{cases}$$ \quad (5.42)

Figure 5.12 gives an example of effective flame length calculation and its relation to the relative geometry between projected flame front and constraints. In this figure, the geometry of flame is fixed and only $x$ is the varying parameter. The $x$ is representing the distance between the injector and Plane C, as defined in Figure 5.9. The relative geometry between constraints and projected flame front is also shown. It can be seen that as $x$ increases, the effective flame length increases due to the center of projected flame front is getting away from the cylinder head and surrounding flame front, which are the two major constraints when Plane C is not far away from the injector. As $x$ keeps increasing, the effective flame length reaches its maximum value at $x = 50\text{mm}$ and then starts to decrease due to Plane C is entering the hemisphere region of the flame and the radius of casted flame surface $r_c$ starts to decrease.
Figure 5.13 shows an example of computed effective flame length $l_x$ as a function of distance between Plane C and injector $x$ and the evolving status of the flame front $r - r_0$. In this condition the piston position is fixed for all cases and $r - r_0$ is the only varying parameter. Figure 5.5 have shown the definition of $r - r_0$, which indicates how far the flame front has traveled compared to the initial condition. As can be seen in Figure 5.13, as the flame front evolves into space, the interaction between flame front and constraints
including cylinder head, piston and surrounding flame fronts varies and the details are captured by the model.

Figure 5.13 An example of computed effective flame length $l_x$ as a function of $x$ and $r - r_0$.

Once the effective flame surface length $l_x$ is evaluated at each Plane C, the total flame surface area $A$ can be obtained by integrating $l_x$ along the spray axis:

$$A = \int_0^{x_t} 2l_x ds$$

(5.43)

where $x_t$ represents the furthest location of Plane C relative to injector as defined in Equation (5.32). The $ds$ can be represented as a function of the Plane C location $x$. For conditions when Plane C is in the cone region ($x \leq x_0$) or hemisphere region ($x > x_0$), $ds$ is represented as:

$$ds = \begin{cases} 
\frac{r}{\cos \theta} dx; & x \leq x_0 \\
\frac{r}{r_x} dx; & x > x_0 
\end{cases}$$

(5.44)
Figure 5.14 gives a schematic description of the iterative computing process of flame front area. Two loops are contained in this iterative scheme: the main loop and the sub loop. The main loop updates the integrated flame area A while the sub loop updates the solution of effective flame surface length $l_x$ at each cycle. The main loop starts by assuming the distance between Plane C and injector $x$ is 0 and ends when Plane C reaches its maximum distance $x = x_t$. Inside the main loop, at each step the coordinates of A, B, C, D, E, O defined in Figure 5.9 are calculated and are used to derive the length of OA, OB, OC, OD, OE. The $l_1$ and $l_2$ defined in Figure 5.11 are subsequently obtained using Equations (5.33) and (5.34). The sub loop starts here by assuming the $x_c$ defined in Figure 5.11 is at its boundary condition $x_c = -r_x$ and ends when $x_c$ reaches another boundary $x_c = r_x$. Inside the sub loop, $y_l$ and $y_c$ defined in Figure 5.11 are calculated according to Equations (5.39) and (5.40) in each step. The relative relation between $y_l$ and $y_c$ is evaluated and the discrete segment of effective flame length $dl_x = f(x_c)$ is determined by Equation(5.42). The $f(x_c)$ is integrated in each iteration of the sub loop and a solution of $l_x$ is reached when $x_c$ reaches boundary condition $x_c = r_x$. The calculation then exits the sub loop and returns to the main loop, where $l_x$ is integrated in each iteration of the main loop following Equation(5.43). The final value of flame surface area A is obtained when Plane C reaches its terminal position $x = x_t$. 
Initial Formation of NG Flame Front

The flame front area calculation scheme assumes the flame initiates from the outer boundary of diesel spray, thus it would cause a step change of flame surface area at start of NG combustion. However, according to the work of Karim et al.[9], the combustion of NG gas in a dual-fuel engine initiates from the multiple ignition sites surrounding the diesel spray. Instead of a step change from 0 to an initial value
determined by the surface area of a diesel spray, the evolving of flame front area at initial stage of NG combustion should be a continuous process. In this work, a method is proposed to approximate the multi-site ignition of NG-air mixture at initial stage of NG flame propagation. The proposed approach assumes ignition sites distribute evenly around the outer boundary of diesel spray and these sites ignites simultaneously at SOC. Upon ignition, individual flame fronts starts to form at each site and propagates freely into the space. The flame is not allowed to travel into the diesel spray thus the flame fronts are approximated as hemispheres.

Figure 5.15 shows the geometrical assumption made at initial stage of NG combustion. The figure is showing a segment from the surface area of a diesel spray. The dots are representing the ignition sites, which are distributed evenly in the surface. The circle around each ignition site represents the flame front evolved from each site. The radius of the hemispherical flame front is defined as \( r \) while the distance between neighbouring ignition sites is defined as \( d \). The flame evolving process during the initial stage of NG combustion is divided into three stages: free evolving, interaction and merging. The free evolving stages include the flame propagation from the ignition site \((r = 0)\) to the point where flame fronts start to interact with each other \((r = d/2)\). The flame propagation then enters the interaction stage when flame fronts interacts and partially merge with surrounding flames. When the flame evolves to a certain stage \((r = d)\), it is assumed that those flame fronts evolved from individual ignition sites merge as a uniform flame front and the flame propagation follows the scheme given the previous sections.
To obtain a numerical solution of the total flame front area in the initial NG combustion stage, the surface area of the igniting diesel spray need to be known. Figure 5.16 gives a 2-D illustration of the approximated diesel spray at SOC. Since diesel spray travels a certain distance before it breaks up into droplets, the surface area shown in this figure does not all contribute to the ignition of the surrounding NG. Instead, the shaded area in this figure is not considered as ignition sites.
In the geometry defined in Figure 5.16, the diesel spray breakup length \( l_b \) can be obtained from Equation (4.6) by setting \( t = t_b \). The definition of other parameters are the same as defined in Figure 5.5. The igniting diesel spray surface area is arrived as:

\[
A_{ini} = 2\pi r_0^2 + \pi r_0 \sqrt{x_0^2 + r_0^2} - \pi l_b \tan \theta \sqrt{l_b^2 + (l_b \tan \theta)^2}
\]  

(5.45)

Based on the assumption that the NG ignition sites distribute evenly along the diesel spray igniting surface, the number of ignition sites from a diesel spray is approximated as:

\[
N = \frac{A_{ini}}{d^2}
\]  

(5.46)

The surface area of each flame front initiated from individual ignition site \( A_0 \) can be determined as a non-continuous functions of flame radius \( r \):
The total flame surface area during the initial stage of NG combustion can be obtained as:

\[ A = A_0 N \]  

(5.48)

Once the flame radius of individual flame front \( r \) reaches the merging point \( r = d \), it is assumed that all individual flames merges as a uniform flame front and the calculation of flame front area follows the iterative scheme given in Figure 5.14.

**Knock Model**

In this work, a reduced 6-step reaction mechanism for prediction the autoignition of NG-air mixture developed by Li et al. [127] is used for the prediction of knock in a dual-fuel engine. Since methane is the major constituent of NG (>90% mass fraction), this work only tracks the reaction between \( \text{CH}_4 \) and oxygen in the end gas zone. The species concentration and end gas zone temperature are used to determine knock. The chemical reaction between methane and oxygen in a dual-fuel engine can be summarized as a reduced 6-step mechanism consisting following reactions:
The reaction rates \( \omega \) of the chemical reactions given above can be represented as a product of reactant concentrations and reaction constant \( k \). The reaction constant of the above reactions are represented in a form of:

\[
k = BT^m e^{-E/RT}
\]

(5.50)

where \( T \) is end gas temperature, \( R \) is ideal gas constant and \( B, m, E \) are rate parameters for each reaction. The rate parameters are summarized in Table 5.1.

Table 5.1. Rate parameters of the reduced 6-step reaction mechanism [128, 129].

<table>
<thead>
<tr>
<th>Reaction No.</th>
<th>( B )</th>
<th>( m )</th>
<th>( E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.98E+13</td>
<td>0.00</td>
<td>238.0</td>
</tr>
<tr>
<td>2</td>
<td>9.04E+12</td>
<td>0.00</td>
<td>103.1</td>
</tr>
<tr>
<td>3</td>
<td>1.60E+07</td>
<td>1.83</td>
<td>11.6</td>
</tr>
<tr>
<td>4</td>
<td>3.30E+11</td>
<td>0.00</td>
<td>37.4</td>
</tr>
<tr>
<td>5</td>
<td>3.90E+10</td>
<td>0.89</td>
<td>1.7</td>
</tr>
<tr>
<td>6</td>
<td>1.20E+17</td>
<td>0.00</td>
<td>190.4</td>
</tr>
</tbody>
</table>

Based on the 6-step reaction mechanism, the change rate of species concentration in the end gas zone can be determined as:
\begin{align*}
  \frac{d[CH_4]}{dt} &= -\omega_1 - \omega_2 - \omega_3 \\
  \frac{d[O_2]}{dt} &= -\omega_1 - \omega_4 - \omega_5 \\
  \frac{d[H_2O]}{dt} &= \omega_2 - \omega_6 \\
  \frac{d[HO_2]}{dt} &= \omega_1 - \omega_2 + \omega_5 \\
  \frac{d[CH_3]}{dt} &= \omega_1 + \omega_2 + \omega_3 - \omega_4 \\
  \frac{d[OH]}{dt} &= -\omega_3 + \omega_4 - \omega_5 + 2\omega_6 \\
  \frac{d[CH_2O]}{dt} &= \omega_4 - \omega_5 \\
  \frac{d[H_2O]}{dt} &= \omega_3 + \omega_4 \\
  \frac{d[CO]}{dt} &= \omega_5
\end{align*}

Auto-ignition of NG can be determined by tracking the species concentration of each reactant in the end gas zone. When a sudden decrease of CH$_4$ concentration and a rise of end gas zone temperature is observed, it is considered as a knocking condition.

**Thermodynamic Model and Gas Properties**

The thermodynamics model used for Quasi-D dual-fuel combustion model is based on the same energy conservation framework discussed in the previous chapter. The heat transfer is addressed differently for dual-fuel combustion. In this work, only convective heat transfer is considered and radiative heat transfer is omitted due to reduced soot production in dual-fuel engines.

The gas composition and property model has also been discussed in the previous chapter. It tracks the species of intake gas, burned products and fuel in each control volume defined by the combustion model. The tracked gaseous species include O$_2$, N$_2$, CO$_2$, H$_2$O, diesel fuel vapor and NG. The concentration of O$_2$, CO$_2$ and H$_2$O are determined from 1), the initial composition of gas, which is a function of EGR ratio and
Mathematical form of the gas property model for \( \text{O}_2, \text{N}_2, \text{CO}_2, \text{H}_2\text{O} \) is given in Equations (5.52) and (5.53), where specific heat capacity \( c_p \) and enthalpy \( h \) are represented as algebraic functions of the temperature in the control volume. The coefficients \( \alpha_1 \) to \( \alpha_6 \) for each species are given in the appendix[119].

\[
\frac{c_p}{R} = \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \tag{5.52}
\]

\[
\frac{h}{RT} = \alpha_1 + \frac{\alpha_2}{2} T + \frac{\alpha_3}{3} T^2 + \frac{\alpha_4}{4} T^3 + \frac{\alpha_5}{5} T^4 + \alpha_6 \frac{1}{T} \tag{5.53}
\]

For diesel vapor and NG, the gas properties are calculated as:[33]

\[
\frac{c_p}{R} = \alpha_1' + \alpha_2' T + \alpha_3' T^2 + \alpha_4' T^3 + \alpha_5' \frac{1}{T^2} \tag{5.54}
\]

\[
\frac{h}{RT} = \alpha_1' + \frac{\alpha_2'}{2} T + \frac{\alpha_3'}{3} T^2 + \frac{\alpha_4'}{4} T^3 - \alpha_5' \frac{1}{T^2} + \alpha_6' \frac{1}{T} \tag{5.55}
\]

where coefficients \( \alpha_1' \) to \( \alpha_6' \) for diesel vapor and NG are provided in the appendix.

**Conclusions**

In this work, a Quasi-D multi-zone dual-fuel combustion model is proposed. The modeling approach used in this work is a combination of the turbulent flame propagation modeling and diesel spray-combustion modeling. Two combustion models runs in parallel to provide a complete prediction of the dual-fuel combustion process. This model applies to the high pressure part of the cycle from IVC to EVO. The diesel spray-combustion model is activated after SOI. After the ignition delay period, the ignition of
diesel spray then triggers both diesel and NG combustion models. The ignition delay correlation includes a pseudo-$\phi$ term, to reflect the realistic diesel fuel to air ratio in a dual-fuel engine.

The diesel combustion model is based on the framework proposed by Hiroyasu et al. which divides the spray into multiple packets, each packet tracks the air and NG entrainment, fuel evaporation and reactions between both fuels and oxygen. The NG combustion model follows the turbulent flame propagation modeling approach originally proposed for SI engines. The way NG is ignited and flame propagates differs greatly from conventional SI combustion. In this work, a new way of modeling the flame front area of NG flame propagation is proposed. The flame is assumed to initiate from the outer boundary of diesel spray, where flamelets initiated from multiple ignition points evolve and merge as a unit flame front. It then propagates freely into the space in the direction perpendicular to the diesel spray boundary and interacts with constraints including cylinder head, wall, piston and surrounding flame fronts. The proposed flame surface area algorithm solves the flame area iteratively in each main iteration of the combustion model. The algorithm incorporates geometrical information of all constraints and it can be a universal solution for various piston or cylinder head design.
CHAPTER SIX

APPLICABILITY AND VALIDATION OF THE QUASI-D DUAL-FUEL COMBUSTION MODEL

Model Validation with Experimental Data

Experimental investigation has been conducted on a chassis dynamometer with a Cummins ISX 550 dual-fuel engine mounted in the class 8 HD truck. The experimental setup has been discussed in detail in Chapter 3.

Due to limited access to measurement of injection pressure and injection rate, a simplified correlation is developed to generate fuel injection rate information as model input. To describe the profile of fuel injection rate, an injection rate shaping array $A_s$ is introduced as a governing parameter. The shaping array $A_s$ is a $[1 \times n]$ array which defines the history of injection rate during the injection event. An assumption is made that $A_s$ remains constant for all injection conditions. With inclusion of shaping array $A_s$, the injection rate can be expressed as:

$$m = \frac{A_s m_{inj}}{\Delta t \cdot \sum_{i=1}^{n} A_s[i]}$$  \hspace{1cm} (6.1)

where $m_{inj}$ total injected diesel mass and $\Delta t$ is a time constant determined by the injection duration. In this work, a symmetric injection profile with gradual increase and decrease of injection rate at the beginning and ending stages is used to approximate the injection characteristics of a unit injector. Figure 6.1 gives an example of the approximated injection rate model. In this figure $A_s$ is fixed as constant for all cases while injected mass and injection duration is varying. It is shown that for a given $A_s$,
when injected mass and injection duration are known, a complete profile of fuel injection rate can be obtained.

In the experiment setup used in this work, the total injected mass $m_{inj}$ is known while injection duration is unknown. However, a correlation between injected mass and injection duration in crank angle basis can be obtained. Thus, the injection duration can be derived from injected mass and a full profile of fuel injection rate can be obtained by applying Equation (6.1). The experimental data of diesel only operation points is used to derive the correlation between injected mass and injection duration. In a conventional diesel engine, the end of injection generally corresponds to the peak of heat release. To obtain a more accurate and consistent detection of EOI, the Quasi-D combustion model is used at diesel only condition is used to infer the injection duration. The performance of the Quasi-D diesel combustion model have been validated in Chapter Five. For each
operating condition, an initial guess of EOI which corresponds to the peak heat release rate derived from cylinder pressure data is used as input for the combustion model. The EOI is then manually tuned to arrive a best fitting of heat release profile.

Figure 6.2 gives an example for the derivation of EOI at engine speed of 1400rpm. Four engine load conditions are used where injected fuel mass per cycle varied between 95 to 225mg. The figure shows the results of using the combustion model to derive the injection duration. Good agreements between model predicted and experimentally derived heat release rates are achieved through the load points.

![Heat release profiles](image)

Figure 6.2 Derivation of EOI by matching the experimentally derived heat release profiles using the diesel only combustion model.
The same method was applied to other engine speeds. A correlation between injection duration and injected mass is then derived through linear regression. Figure 6.3 shows the derived injection duration as a function of injected mass. A clear linear relationship was observed with $R^2 = 0.974$. The correlation between injection duration in crank angle degree $CA_{inj}$ and injected mass $m_{inj}$ is arrived as:

$$CA_{inj} = 0.124m_{inj} + 4.815$$  \hspace{1cm} (6.2)

where $CA_{inj}$ is in deg and $m_{inj}$ is in mg. Once the injected mass per cycle is known, the injection duration can be obtained from this correlation and a full profile of mass injection rate can be arrived subsequently. This approach also applies for dual-fuel operation conditions.

The Quasi-D combustion model is validated with experimental data for both diesel only and dual-fuel conditions. At diesel only condition, the model inputs associated
with NG are set to zero and only the diesel spray-combustion model is activated. The injection duration and rate correlations given in the previous section are used to generate inputs with regard to diesel injection. Figure 6.4 gives the validation results of diesel only operation conditions where heat release and cylinder pressure are used for validation. Two engine speeds and four load conditions are tested. It is shown that the model agrees well with experimental data at various engine operating conditions. Though at higher loads the model is losing some details of heat release rate when the heat release is around its peak, the cylinder pressure prediction still agrees well with experimental data.
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Figure 6.4 Validation results of heat release profile and cylinder pressure at diesel only operation conditions

Figure 6.5 gives the validation results of dual-fuel operating conditions. Two examples are given here where engine speeds are both 1200rpm but engine load and NG substitution ratio is different. The percentages of NG in energy content are 65.6% and 31.8% respectively. Figure 6.5 a(1) and a(2) show the comparison between model predicted and experimentally measured and derived cylinder pressure and heat release rate, while Figure 6.5 b(1) and b(2) show the modeled heat release rate contributed from both diesel and NG. The injection duration derived from the correlation developed in the previous section is also shown here as reference. It can be seen from the figures that though the heat release profile of these two operating conditions are alike, the contributions from combustion of NG and diesel fuel are quite different. It is shown from Figure 6.5 b(1) and b(2) that the proposed diesel injection duration correlation output
reasonable injection profiles at dual-fuel conditions and enables accurate prediction of heat release rate.

The turbulent flame propagation model and diesel spray combustion model work simultaneously to output the energy released by both fuels. The energy fraction of both fuels are represented in the heat release rates predicted by the model. Overall the model agrees very well with experimental data in terms of both heat release rate and cylinder pressure.
Figure 6.6 shows the predictions of NG flame front surface area of the same engine operation conditions shown in Figure 6.5. The flame surface area $A_{\text{flame}}$ and propagation distance $R_{\text{flame}}$ are normalized with the square of bore and bore, respectively. The traveled distance $R_{\text{flame}}$ is the same as $r - r_0$ in the geometry definitions given in Figure 5.5. It is shown that the flame front surface area model captures well the details of the flame evolving history in its initiation, free-evolving and constraint cut-off stages. The difference between flame surface area evolving histories obtained for the two operating conditions is mainly due to the penetration length of the diesel spray at SOC. For the higher load case (IMEP = 19.8bar), the ignition delay is shorter compared to the lower load case, resulting a shorter penetration length, and a smaller surface area to initiate the combustion of NG-air mixture. Therefore, in the early
free-evolving stage, the normalized flame surface area of the higher load case is lower than at lower load. The higher load case has a higher normalized flame propagation distance $R_{\text{flame}}$ at the end of combustion, due to the shorter diesel spray penetration at the initial condition.

Figure 6.6 Model prediction results of NG flame front surface area

![Graph showing model prediction results](image)

Figure 6.6 Model prediction results of NG flame front surface area

Figure 6.7 shows the comparison between model predicted diesel spray tip penetration length and NG flame propagation distance. This figure shows the relative position between the diesel spray and NG flame front. The distances shown in the figure are relative distances between spray tip and injector, and between flame front (on the spray axis) to the injector. It can be seen that after start of combustion, the diesel spray tip travels further than the NG flame front, which indicates that the diesel spray reaches the wall before the NG flame does. Ideally, the change in air entrainment of diesel spray, as well as the entrainment rate and flame front area of the NG flame as a function of relative
spatial position between the spray tip and NG flame front need to be incorporated in the model. For simplicity reason and the concern of computational load, these effects are neglected in this work.

Figure 6.7 Comparison between diesel spray tip penetration and NG flame propagation distance at a typical operating condition. The distances shown in the figure are relative distances between spray tip and injector, and between flame front (on the spray axis) to the injector.

![Figure 6.7](image)

Figure 6.8 a(1) and b(1) shows the model prediction results of in-cylinder temperatures, including the unburned gas temperature, burned gas temperature and bulk temperature. The unburned zone includes the gas that is not involved in the combustion, while the burned gas temperature is the average temperature of burned gas generated by the combustion of both diesel and NG. Figure 6.8 a(2) and b(2) show the temperature predictions for different packets. The $i_{pac}$ in the legend denotes the index of packet on
the $x$ axis. In this case the total number of packet sets on the $x$ axis (packets with same $x$ index) is 20. This figure shows the predicted temperature history in individual packets, where packets with smaller $i_{pac}$ are injected earlier than the packets with larger $i_{pac}$. This displays the fidelity of the model that the temperature distribution within the spray can be captured, which provides more insight for studies of emissions compared to the models that use single burned zone to represent the diesel spray. The packet temperature model together with the spray penetration model can also provide spatial resolution of temperature distribution within the spray.
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Parametric Studies

This section investigates the fidelity and predictiveness of the model by conducting parameter sweeps. The case studies include a basic engine operation parameter sweep, a knock study and an unburned NG study.

Engine Actuator Sweep

The tested matrix for in the engine actuator sweeps is summarized in Table 6.1. The investigated parameter sweeps include NG substitution ratio, total equivalence ratio and diesel SOI. These are the three parameters that have the most profound effect on the combustion characters in a dual-fuel engine, and ultimately define the acceptable operating range. The quasi-D combustion model developed in this work is expected to
have the fidelity to predict the change in the combustion characters resulted from the change of those governing parameters.

The baseline engine operation condition is engine speed of 1200rpm, NG substitution ratio at 60%, total $\phi$ at 0.6 and SOI at -4.5 degATDC. For each parameter sweep, only one parameter is varied while others are maintained the same as baseline condition.

Table 6.1. Simulation parameters for engine actuator sweeps.

<table>
<thead>
<tr>
<th>NG %</th>
<th>Total $\phi$</th>
<th>SOI degATDC</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.6</td>
<td>-5</td>
</tr>
<tr>
<td>40</td>
<td>0.6</td>
<td>-5</td>
</tr>
<tr>
<td>60</td>
<td>0.6</td>
<td>-5</td>
</tr>
<tr>
<td>80</td>
<td>0.6</td>
<td>-5</td>
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<td>60</td>
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<tr>
<td></td>
<td>0.6</td>
<td>-7.5</td>
</tr>
<tr>
<td></td>
<td>0.8</td>
<td>-10.5</td>
</tr>
</tbody>
</table>

Figure 6.9 shows the simulation results of NG substitution ratio sweep. Three predicted variables including heat release rate from both fuels, cylinder pressure, bulk gas temperature. Figure 6.9(a) shows the prediction of heat release rate from both fuel with various NG substitution rate and diesel fuel injection rate. The fuel injection rate is multiplied by 5 in unit of mg/CA. It is clearly shown that with higher NG%, the heat release contribution from NG becomes more dominant, while the diesel injection duration and heat released from the combustion of diesel fuel decreases. Since the total $\phi$ for each
case is the same, the total heat release profiles are similar, with variation in phasing due to the difference of burn rate between the two fuels. Figure 6.9(b) shows the predicted cylinder pressure. The cylinder pressure profiles for each case are similar due to the same total $\phi$, but slight variations of peak cylinder pressure are observed. With NG% increased from 20% to 60%, the peak cylinder pressure increases due to the higher heating value of NG compared to that of diesel. However, when NG% reaches 80%, the peak cylinder pressure is lower than in the case of NG% = 40%. This is due to the incomplete combustion of NG at higher NG substitution rates, which will be discussed in detail in later sections. Figure 6.9(c) shows the prediction of bulk in-cylinder gas temperature. The trend is similar to what was discussed related to the cylinder pressure prediction.
Figure 6.9 Simulation results of NG substitution ratio sweep. (a) Heat release rate; (b) Cylinder pressure (c) Bulk gas temperature

Figure 6.10 shows the simulation results obtained for a sweep of total $\phi$.

Equivalence ratio $\phi$ varied from 0.2 to 0.8 in the tested cases while NG% maintains at 60%. Figure 6.10(a) shows the prediction of heat release rate from both fuels and diesel fuel injection rate, for selected values of total $\phi$. It is clear shown that as total $\phi$
increases, total heat release rate increases correspondingly, while the relative portion of heat release contributed from both fuels remains consistent in all cases. Due to the increased total $\phi$, thus increased heat released into the cylinder charge, Figure 6.10(b) and (c) both shows elevated cylinder pressure and temperature with higher total $\phi$. 
Figure 6.10 Simulation results obtained from a range of total \( \phi \). (a) Heat release rate; (b) Cylinder pressure (c) Bulk gas temperature

Figure 6.11 shows the simulation results for the SOI sweep. The SOI varied from -1.5 to -10.5 degATDC, while NG\% was maintained at 60\%, and total \( \phi \) at 0.6. Figure 6.11(a) shows the prediction of heat release rate from both fuel with various injection timings. The diesel injection profile is the same for all cases since injection timing is the only variable parameter. It can be seen from this figure that combustion characters change vastly. With advanced injection timing, a longer ignition delay and a higher peak heat release rate are observed. The cylinder pressure and temperature prediction given in Figure 6.11(b) and (c) both reflect the effect of heat release shown in Figure 6.11(a). With retarded injection timing, both peak cylinder pressure and temperature are reduced. In Figure 6.11(c), a reduction of nearly 250K of temperature is achieve with 9 deg retarded injection timing. Meanwhile, the torque output as well as thermal efficiency can be expected to deteriorate with retarded SOI, judging from the cylinder pressure
predictions. These insights can be used for investigations of injection strategies for dual fuel engines with emphasis on either performance or emissions.
Knock Study

The knock model used in this work is based on a reduced chemical mechanism extensively calibrated in dual-fuel engine literature[127]. The model was presented in Chapter 5. Due to the limited experimental data sets, knocking conditions were not tested specifically in the experiments. Rather than validating the predictiveness of the model with experimental knock data, the purpose of this section is to investigate the fidelity of the knock model and its sensitivity to the inputs. The knock model is expected to capture the effects from the change of key parameters that affect the knock, including compression ratio, intake gas temperature and engine load or total equivalence ratio.

Figure 6.12 shows the simulation results of the knock model in a non-knocking engine operating condition. The engine operates at 1200rpm at IMEP of 16.1bar with NG substitution rate of 65%. This figure shows the history of species concentration and gas
temperature in the end-gas zone. The temperature profile shown in this figure is multiplied with a constant of 1E-10 for reference. It can be seen that at non-knocking condition, the species concentration of CH$_4$ remains the same as initial condition while the concentration of products including OH, CH$_3$ etc. remains as zero. This indicates no autoignition has occurred during the entire combustion process, and this can be considered a non-knocking condition.

It is well known that the occurrence of knock largely depends on the temperature of the end-gas. To investigate sensitivity of the model, initial gas temperature is elevated by 10%. The simulation results are shown in Figure 6.13, where a sudden change of concentration of CH$_4$ and products, as well as end gas temperature, occurred at around CA = 20degATDC. The concentration of CH$_4$ quickly drops to zero, along with a sharp increase of end gas temperature, which indicates autoignition. Therefore it is considered that knock has occurred. Figure 6.13(b) gives a zone-in view of the autoignition process. The knock model predicts the change of species concentration as well as the end gas
temperature. This demonstrates the fidelity of the knock model based on the chemical reaction mechanism. In comparison to empirical knock models, such as the Arrhenius function based correlations, this model not only provides the prediction for onset of knock, but also generates the information about species concentration and temperature. This information can in turn provide inputs for estimating cylinder pressure.
Figure 6.13 Knock model simulation results of end-gas temperature and species concentrations: Knocking case. (a) Normal view (b) Zone-in view

Figure 6.14 demonstrates the predictiveness of the knock model. Figure 6.14(a) shows cylinder pressure profiles from experimental injection timing sweep. It is shown that as injection timing advances, peak cylinder pressure rises. When injection timing is advanced to a certain point, knock starts to occur. The timing information shown in the legend indicates the injection timing pulse width, which has been discussed in Chapter 3. Figure 6.14(b) shown the model prediction results of the same operating condition. It is shown that with advanced injection timing, the model accurately reproduces the change of peak cylinder pressure. When the injection timing is advanced to -12degATDC, knock is automatically predicted by the model, which matches well with experimental data.
To further investigate the fidelity and predictiveness of the knock model, parameter sweeps including initial gas temperature, compression ratio and total $\phi$ are conducted. These three parameters all have strong effects to engine knock, and it is critical to assess the ability of the knock model to capture these effects. Table 6.2 summarizes the simulation parameters for the parametric study of the knock model predictions. The baseline condition is at 1200rpm, initial gas temperature at 400K, compression ratio of 17 and total $\phi$ at 0.8. In each parametric sweep, only one parameter is being changed while all other parameters maintain the same value as the baseline conditions.

Table 6.2. Simulation parameters for knock study.

<table>
<thead>
<tr>
<th>Initial Temperature (K)</th>
<th>Compression Ratio</th>
<th>Total $\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>380</td>
<td>17</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Figure 6.14 Knock model validation with experimental injection timing sweep. (a) Experimental data (b) Simulation
Figure 6.15 show the knock model predicted end-gas temperatures for various initial temperature conditions. It can be seen that at initial temperature $T_{ic} = 380K$, no sudden change occurs to the end-gas temperature, which indicates a non-knocking condition. When $T_{ic}$ increases over 400K, sudden rise of end-gas temperature is observed close to TDC, which indicates onset of knock. As $T_{ic}$ increases, the onset of knock advances due to elevated chemical reaction rates.
Figure 6.15 Knock model simulation results of initial gas temperature sweep

Figure 6.16 shows the knock model predicted end-gas temperature for various engine compression ratio. At baseline condition CR = 17, the model predicts knock at CA = 22degATDC. It can be seen from the figure that with lower compression ratio CR = 16, the onset of knock is retarded around 5 deg. With even lower compression CR = 15, no knock would occur. On the contrary, with elevated CR, the onset of knock advances. This is due to the change of in-cylinder gas temperature and pressure histories, and these effects are well captured by the model.
Figure 6.16 Knock model simulation results for a compression ratio sweep

Figure 6.17 shows the knock model predicted end-gas temperature for a range of total $\phi$. The total $\phi$ is a parameter that represents the engine load. It is generally agreed that higher load condition is more favorable for knock to occur, due to elevated end gas temperature and pressure during combustion. It can be seen from the figure that at baseline condition when total $\phi$ is 0.8, knock occurs at 22 degATDC. As engine load decreases, the onset of knock retards, and until eventually it ceases to occur. On the other hand, if the engine load keeps increasing, the onset of knock advances.
The knock model developed in this work is a useful tool for engine researchers to understand operation limits and to expedite engine calibrations. Even though the accuracy of the model is not validated with experimental data, its sensitivity to key input parameters agrees with research work from others. When detailed experimental data is available, this model can be easily calibrated to output reliable prediction results.

Incomplete NG Combustion Study

As has been discussed in the review chapter of dual-fuel engines, the two major limiting factors are knock and methane slip. The previous section discussed the model predictiveness with respect to knocking conditions. In this section, a parametric study is conducted to investigate the model’s ability to predict incomplete NG combustion.

The two major parameters that would affect the incomplete NG combustion in a dual-fuel engine are NG substitution ratio and engine load. Table 6.3 summarizes the simulation parameters for the parametric study of incomplete NG combustion. The
baseline condition is at engine speed of 1200rpm, NG substitution ratio at 60%, compression ratio of 17 and total $\phi$ at 0.6. In each parametric sweep, only one parameter is being changed while all other parameters maintains the same as the baseline conditions.

Table 6.3. Simulation parameters for a study of incomplete NG combustion.

<table>
<thead>
<tr>
<th>NG%</th>
<th>Total $\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.6</td>
</tr>
<tr>
<td>40</td>
<td>0.2</td>
</tr>
<tr>
<td>60</td>
<td>0.3</td>
</tr>
<tr>
<td>80</td>
<td>0.4</td>
</tr>
<tr>
<td>90</td>
<td>0.6</td>
</tr>
<tr>
<td>60%</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Figure 6.18 shows predictions of NG MFB for NG substitution ratio and engine load sweeps. It is shown that NG combustion efficiency tends to deteriorate with increase of NG% and decreased engine load. Figure 6.19 further illustrated NG combustion efficiency as a function of NG% and engine load. At a fixed total $\phi$ condition, an interesting phenomenon is found. The maximum NG combustion efficiency is achieved with 40% NG substitution ratio instead of 20%. This is because as NG% becomes very low (20%), the equivalence ratio of NG is small, resulted in a reduced laminar flame speed, see Equation(5.12), hence a longer time is needed to consume all the NG. As the NG substitution ratio increases, energy released from the combustion of diesel fuel decreases, hence a less powerful ignition source is available for the NG-air mixture,
resulting a reduced combustion efficiency. For the NG substitution ratio sweep, even at the worst condition, the NG combustion efficiency is still over 95%. The engine load sweep on the other hand, a NG combustion efficiency below 90% is observed for $\phi = 0.2$. The reduction of NG combustion efficiency at low load conditions are due to reduced NG laminar flame speed as well as the ignition energy released from diesel fuel.
Figure 6.18 Predictions results of NG MFB with various (a) NG substitution ratios and (b) engine load conditions.

![Graph](image)

Figure 6.19 Summary of NG combustion efficiency as a function of (a) NG substitution rate and (b) engine load.

Conclusions

In this Chapter, the Quasi-D multi-zone dual-fuel combustion model is validated with experimental data. Its fidelity and potential usage are demonstrated as well. Due to limited access to injection measurements, a correlation is developed to infer the diesel fuel injection profile. A linear correlation was found between injected mass and injection duration with diesel only operation. The correlation was subsequently used to estimate
injection duration from injected mass and is also applied to dual-fuel operating conditions. The dual-fuel combustion model is validated with experimental data for both diesel only and duel-fuel operations. The model displays good agreement with experimental data in both heat release and cylinder pressure at various operating conditions. The model also generate valuable information that is difficult to be measured such as the in-cylinder temperature and heat release contributed from each fuel. The model also has the fidelity to predict the temperature in each packet of the diesel spray, which provides valuable information for the studies of temperature-dependent emissions. Parametric studies including engine load, substitution ratio and SOI sweeps have demonstrated the sensitivity of the model to the engine operating parameters. Simulation studies with regard to knock and incomplete NG combustion further demonstrate the capability of the model.

This work has provided a throughout description of a Quasi-D dual-fuel combustion modeling scheme that can easily be used by other researchers. By varying the number of packets and calculation time step, a balance between computing power requirement and model fidelity can be reached based on the simulation goal. The model can help expedite the calibration or development process of a dual-fuel engine, and can also be used for investigating new dual-fuel combustion concepts.
CHAPTER SEVEN
INTAKE CHARGE ESTIMATION MODEL

Introduction

In this work, the gas exchange model is developed based on a SI engine platform. An SI engine generally requires stricter AFR control accuracy compared to that of a CI diesel or a dual fuel engine because the three way catalyst requires engine to operate at stoichiometry to reach its maximum efficiency. While dual fuel engines on the other hand, can operate with a wide range of equivalence ratio. An accurate estimation of air charge is still critical for controlling engine transient response and emissions. An over-lean condition would lead to excessive production of NOx emission and contribute to incomplete NG combustion, while an over-rich condition will result in production of soot as well as unburned fuel. Additionally, an accurate prediction of intake air charge is a critical input for the combustion model since the combustion model need the knowledge of charge composition as initial conditions.

The objective of the in this Chapter is to develop a universal feedforward air charge estimation approach which requires little or no calibration effort, while maintaining the prediction accuracy under both steady-state and transient conditions. Real-time predictions are a must with an original approach proposed in this Chapter. Previous researchers have investigated this topic and developed multiple solutions. The instantaneous air mass flow at the intake valve is hard to measure directly, thus various estimation techniques have been developed to estimate air charge using measurements from sensors at other locations. Generally, previous work and state-of-the-art production
systems can be categorized into two groups, the Mass Air Flow (MAF) meter based, and Speed-density systems. Both have deficiencies that will be addressed.

**Background**

Mean value models are widely used in modeling the dynamics of the air path due to its low requirement of computation effort. Figure 7.1 shows the typical setup for the mean value model of the intake air path, where $m$ depicts mass, $p$ depicts pressure, $T$ depicts temperature, $U$ depicts internal energy, $H$ depicts enthalpy and $Q$ depicts heat. The system has a fixed volume where thermodynamics states are assumed to be uniform in the entire volume [130].

![Figure 7.1 Inputs, states and outputs of intake air path.](image)

The inputs and outputs are mass and energy flows. It is assumed that no heat or mass transfers occur between the gas and the wall and no substantial change occurs to the kinetic energy in the flow. Thus the system described in Figure 7.1 can be represented by the following two differential equations:
\[
\frac{d}{dt} m(t) = \dot{m}_{in}(t) - \dot{m}_{out}(t) \tag{7.1}
\]
\[
\frac{d}{dt} U(t) = \dot{H}_{in}(t) - \dot{H}_{out}(t) + \dot{Q}(t) \tag{7.2}
\]

According to ideal gas law and caloric relations, following correlation can be applied to the air path system:

\[
p(t) \cdot V = m(t) \cdot R \cdot T(t) \tag{7.3}
\]
\[
U(t) = c_v \cdot T(t) \cdot m(t) \tag{7.4}
\]
\[
\dot{H}_{in}(t) = c_p \cdot T(t) \cdot \dot{m}_{in}(t) \tag{7.5}
\]
\[
\dot{H}_{out}(t) = c_p \cdot T(t) \cdot \dot{m}_{out}(t) \tag{7.6}
\]

where \(V\) is manifold volume, \(R\) is ideal gas constant, \(c_v\) is constant volume specific heat and \(c_p\) is constant pressure specific heat. The composition of gas is assumed to remain unchanged in this control volume thus \(R, c_v\) and \(c_p\) can be represented as constants.

Substitute Equations (7.3) - (7.6) into Equations (7.1) and (7.2), the intake manifold dynamics can be represented as:

\[
\frac{d}{dt} p(t) = \frac{\gamma R}{V} \left[ \dot{m}_{in}(t) \cdot T_{in}(t) - \dot{m}_{out}(t) \cdot T(t) \right] \tag{7.7}
\]
\[
\frac{d}{dt} T(t) = \frac{R \cdot T(t)}{p(t) \cdot V} \left[ \dot{m}_{in}(t) \cdot (\gamma \cdot T_{in}(t) - T(t)) - \dot{m}_{out}(t) \cdot (\gamma - 1) \cdot T(t) \right] \tag{7.8}
\]

When dwell time of gas in the manifold is small or the surface-to-volume ratio of the manifold is small, adiabatic assumption in Equations (7.7) and (7.8) works well. On the contrary, when large heat transfer occurs in the manifold or the surface-to-volume ratio is large, the inlet gas temperature \(T_{in}\) and the manifold gas temperature \(T\) are
assumed to be the same. Then the isothermal assumption is better approximation.

Equations (7.7) and (7.8) can be rewritten to:

\[
\frac{d}{dt} p(t) = \frac{T(t) \cdot R}{V} \left[ \dot{m}_{in}(t) - \dot{m}_{out}(t) \right]
\]  

(7.9)

\[
T(t) = T_{in}(t)
\]  

(7.10)

The isothermal intake manifold approximation is widely used in engine applications due to its simplicity and better accuracy compared to that of adiabatic approximations [131, 132].

**MAF Based Methods**

MAF based feedforward air charge estimation utilizes a MAF sensor located upstream of the throttle to measure mass air flow rate entering the engine. MAF based approach generally yields very accurate mass air flow estimation in steady-state conditions. The direct measurement of air mass flow automatically includes the lumped effect of engine operating conditions, ambient conditions and the effect of engine aging. On the other hand, MAF based approaches are subject to several limitations. At transient conditions, MAF measurements do not capture the manifold filling/emptying dynamics due its upstream location. Additionally, MAF sensors use hot wire anemometers to measure air mass flow, which has slower sensor dynamics compared to that of a MAP sensor. Finally, MAF sensors are also known for sensor fouling and drifting [133] and the cost of a MAF sensor is higher than a MAP sensor.
Research focused on MAF based air charge estimation methods is largely motivated by a need to address response during transient conditions. Due to the upstream location of sensor, the filling/emptying dynamics of the intake manifold is not being captured by the sensor. Thus a model is required to estimate the true air flow through the intake valve using the sensor measurement as input. Grizzle et al. proposed a nonlinear open-loop air charge observer which uses MAF sensor as input [134]. The intake manifold is modeled using the isothermal approximation described in Equations (7.9) and (7.10), given as:

\[
\frac{d}{dt} p = \frac{TR}{V} [MAF_a - Cyl(N, p)]
\]  

(7.11)

where \( p, T \) and \( V \) are pressure, temperature and volume of the gas in the intake manifold, \( MAF_a \) is the actual air mass flow rate upstream of the manifold and \( Cyl(N, p) \) is the air mass flow rate entering the cylinder represented as a function of engine speed \( N \) and manifold air pressure \( p \). The cylinder pumping or induction function \( Cyl(N, p) \) can be represented as polynomials with coefficients determined from dynamometer data [135]. The dynamics of MAF sensor can be modeled as a first order lag with time constant in the order of 20ms:

\[
\tau \frac{d}{dt} MAF_m + MAF_m = MAF_a
\]

(7.12)

where \( MAF_m \) is the air mass flow rate measured by the MAF sensor located upstream of the manifold and \( \tau \) is the time constant of MAF sensor. Substituting Equation (7.12) into Equation (7.11) yields:
\[
\frac{d}{dt} p = \frac{TR}{V} \left[ \frac{\tau}{dt} MAF_m + MAF_m - \text{Cyl}(N, p) \right] \quad (7.13)
\]

Let \( x = p - (RT/V)\tau MAF_m \), the cylinder air charge per induction event CAC can be represented as:

\[
CAC = \frac{120}{nN} \text{Cyl}(N, x + \frac{RT}{V} \tau MAF_m) \quad (7.14)
\]

where \( n \) is number of cylinders. Experimental results have shown that the above method yielded good AFR control under transient conditions.

**MAP Based Methods**

Another widely used air charge estimation method is the speed-density approach, which uses MAP sensor as one of the primary inputs. The speed-density mass air flow estimation approach is given with the form shown in Equation (7.15), where \( m_a \) is the mass of air entering one cylinder per cycle, \( \eta_v \) is volumetric efficiency, which is represented as a function of engine speed \( N \) and manifold air pressure \( p \). \( \rho_a \) is density of air in the manifold, \( V_d \) is the displacement of each cylinder, \( R \) is ideal gas constant of air and \( T \) is manifold gas temperature.

\[
m_a = \eta_v \rho_a V_d = \frac{\eta_v(N, p_m, \cdots)V_d p_m}{R \cdot T_m} \quad (7.15)
\]

The speed-density approach uses measured manifold air pressure \( p \) from a MAP sensor, manifold air temperature \( T \) and volumetric efficiency (VE) \( \eta_v \) from a calibrated table to estimate mass air flow. This approach has better transient performance compared to MAF based approach since a MAP sensor has fast dynamics. However, the VE table which stores information of VE at various engine operation conditions generally requires
extensive calibration effort. In Equation (7.15), VE is a function of engine speed and MAP, which requires calibration of a two-dimensional table. In case of a high Degree-of-freedom engine, the size of look up tables increases exponentially, as well as the calibration effort.

Jankovic et al. [136] proposed an algorithm that included the effect of EGR on the speed-density based charge estimation by estimating the partial pressure of EGR and subtracting it from measured total manifold pressure. The partial pressure of EGR is estimated as:

$$p_{EGR} = \frac{RT}{V} \left( \dot{m}_{EGR} - \alpha_1(N)p_{EGR} - \alpha_2(N) \frac{p_{EGR}}{p} \right) \quad (7.16)$$

where $p_{EGR}$ is partial pressure of EGR, $\dot{m}_{EGR}$ is the mass flow rate of EGR and $\alpha_1(N)$, $\alpha_2(N)$ are coefficients as functions of engine speed $N$.

As the regulation of fuel consumption and GHG emissions are tightened, auto makers are adopting technologies such as variable valve actuation (VVA), Exhaust gas recirculation (EGR) and turbocharging, which all bring additional degree-of-freedoms, thus adding new dimensions to the VE table. Problems may rise here since the calibration effort is exponential with the dimension of the table. Increased size of map data also requires more ECU memory, both will induce additional costs.

Reducing the calibration effort of VE table in a high DOF engine has been an active research area. Lee et al. [137] has proposed mean value models to compensate the effect of VVT and turbocharging in a SI engine and demonstrated good transient performance. Artificial neural networks (ANN) have also been applied to reduce the
calibration effort of generating VE tables. Wu et al. [138] proposed training ANNs on a large set of engine data, to produce a compact VE model for a high DOF engine. The ANN was trained by steady state dynamometer data, where engine speed, manifold air pressure, exhaust and intake cam timing are used as inputs. The proposed method greatly reduced the calibration effort of a high DOF engine and the performance was validated by both dynamometer test data and in-vehicle test data. Extrapolation can be avoided by introducing the high-fidelity engine system simulation and generating data that covers all realistic points. However, new ANNSs have to be trained in case of hardware changes.

Physics based VE calculations have also been investigated. Turin et al. [139] have proposed a physics based VE model for engines with VVA, where VE is calculated using inputs of MAP, engine speed and cam profiles. Kocher et al. [140] have also investigated physics based VE modeling of diesel engines where VVT, turbocharging and EGR are equipped. The model was validated with dynamometer testing and the modeled VE has achieve less than 5% error compared to the calibrated VE table.

The major differences between MAF bases and Speed density approaches are summarized as: 1) Sensor usage. MAF bases approaches utilize a mass air flow meter upstream of the intake system, typically before the throttle, while Speed density approaches use a manifold absolute pressure sensor located at the manifold. In this case, Speed density approach has its advantage due to lower sensor cost. 2) Transient performance. Due to slow dynamic response of hot wire anemometer used in a MAF sensor, MAF bases approach has poor accuracy during transients, compared to the Speed density approach. Physical models or observers need to be developed to compensate the
intake air mass flow during transient conditions. On the other hand, Speed density approach has better response at transients due to fast pressure measurements. However, the calibration effort associated with VE tables penalizes its application in the case of a high DOF engine.

Other Methods

The air charge estimation methods mentioned above uses either MAF or MAP sensor as sensor input. When both sensors are present in a vehicle, the air mass flow rate entering the cylinder can be represented as:

\[
\dot{m}_a = \dot{m}_{MAF} - \frac{V}{RT} \dot{p}_m
\]

where \(\dot{m}_{MAF}\) is air mass flow rate measured by MAF sensor and \(p_m\) is manifold air pressure measured by MAP sensor. The major challenge of this approach is sensor noise. Jankovic et al. and Leroy et al. have developed combined MAF and MAP based air charge estimation for an engine equipped with turbocharger, variable valve timing (VVT) and EGR [141-143], where various observers are used to estimate the air charge from both sensor measurements.

Other researchers investigated the possibility to estimate air charge mass using measured cylinder pressure. Colin et.al [144] proposed an approach using cylinder pressure to estimate cylinder charged mass and Qu et al. [145] used measured cylinder pressure to realize physics based crank-angle resolved gas exchange estimation. Sensor accuracy and signal noise present significantly obstacles.

The aforementioned air charge estimation methods all strive to obtain an accurate air flow prediction in both steady state and transient conditions. However, most of them
still require extensive experimental calibration effort. Speed-density based approaches all rely on VE tables, which is tied with experimental calibration, unless the VE table is physically modeled [139]. Some approaches use information from cylinder pressure measurement, which induces additional complexity and costs. Additionally, few of these approaches realize crank-angle resolved mass air flow estimation. Most of the approaches lumped the effects during the intake process and estimate value of final charge mass, while the physics phenomenon during the intake period are not captured.

The physics based feedforward air charge estimation algorithm developed in this work has the potential to work across different engine platforms, including those equipped with VVA and EGR. Realization of physics based air charge prediction would greatly reduce calibration cost of the VE table for engines equipped with higher number of actuators. The model can also be used for future development of a combined MAP/MAF based air charge algorithm, which incorporates the benefits of both MAF measurements and physics based feedforward model. In this work, a modeling approach that only uses intake runner pressure as pressure input is developed. A minimal number of sensors is required to avoid installation of an intake runner pressure transducer, a lookup based intake runner pressure model is proposed to generate crank angle resolved runner pressure profile as model input. The real-time air charge prediction algorithm was first tested with a production engine in a dynamometer setup and was subsequently implemented on a test vehicle at a proving ground. To evaluate the cross-platform application potential of the proposed algorithm, the air charge prediction model was implemented to a MultiAir VVA engine. Due to limited access to experimental facility,
only a simulation study of a VVA engine was conducted, but GT-Power simulation was available as baseline for validation. The study conducted using such “virtual engine” has revealed that the proposed air charge prediction algorithm also applies to VVA engines, with some enhancements, including an additional intake runner air temperature model and more detailed information on the exhaust side under certain valve actuation strategies.

**Modeling of Gas Exchange Process**

The gas exchange process plays a key role in an ICE. The gas exchange process determines the following: 1) Mass of air charged into the cylinder, which in turn determines the mass of fuel to be injected and the engine load. 2) Pumping work, which is a key parameter that affects engine efficiency. 3) Internal residual gas fraction (RGF), which affects the combustion characters.

Figure 7.2 shows a schematic diagram of the gas exchange process of a typical internal combustion engine. After completion of combustion, the exhaust valves open and gas exits the cylinder through the exhaust valves with mass flow rate $\dot{m}_{ex}$. Intake valves typically start to open right before the exhaust valves close. During the initial stage of intake valve opening, cylinder pressure may be greater than the pressure upstream of the intake valve, causing a backflow of the residual gas into the runner. As the piston moves from top dead center (TDC) to bottom dead center (BDC), cylinder pressure drops. After the pressures equilibrate, and ultimately the pressure in the cylinder drops below the pressure upstream of the valve, the fresh mixture as well as the burned gas trapped in the
intake runner due to backflow starts to flow into the cylinder with mass flow rate $\dot{m}_{in}$. The convention used in this paper assigns a positive value to flow into the cylinder through either the intake or exhaust valve, and vice versa. The intake valve is typically closed shortly after BDC thereby eliminating the backflow which may occur before the intake valve fully closes due to the upward motion of the piston.

Figure 7.2: Schematic diagram of gas exchange process in an internal combustion engine.

In this Chapter, the primary research focus is on the intake process. The model is expected to predict mass flow across the intake valve during intake valve opening. Although the estimation of intake charge is the primary focus, it cannot be accomplished by just studying the flow through the intake valve. The gas exchange process involves both intake and exhaust dynamics. Flow through exhaust valves can affect the intake,
especially during valve overlap, as shown in Figure 7.3. For illustration purposes, the convention is changed in this figure only, i.e. flow is entering the cylinder when intake mass flow is positive, while it is exiting the cylinder when exhaust flow is positive. It is shown that during the valve overlap it is possible to have simultaneous backflow through the exhaust valve (back into the cylinder) and the intake valve (out of the cylinder), for a very short period of time. Eventually, the regular flow through the intake valve starts to dominate. Differing gas properties at intake and exhaust sides add complexity to model development. Finally, modern engines are typically equipped with variable valve actuators wherein cam timings are adjusted in real time to achieve optimum volumetric efficiency and residual gas fraction. The intake charge crank-angle based flow model needs to be capable of capturing these effects as well.

Figure 7.3. An illustration of gas exchange process near valve overlap stage.
Mathematical Modeling Approach

This section provides a description of the intake flow mathematical model. A 0-D modeling approach was selected to facilitate real-time applications. From the continuity equation, the mass flow rate of an open thermodynamic system is equal to the total mass flow rate in and out of the system:

\[ \dot{m} = \sum_j \dot{m}_j \]  

(7.18)

The gas property in the open thermodynamics system follows ideal gas law:

\[ p = \frac{1}{V} RT m \]  

(7.19)

where \( p \) is pressure, \( V \) is volume, \( T \) is temperature, \( m \) is mass of gas and \( R \) is ideal gas constant.

The mass flow rate across a poppet valve for compressible flow can be written as a function of the pressures upstream and downstream of the valve \( p_u \) and \( p_d \), upstream temperature \( T_u \), valve reference area \( A_R \) and experimentally measured discharge coefficient \( C_d \):

\[ \dot{m} = \frac{C_D A_R p_u}{(RT_u)^{1/2}} \left( \frac{p_d}{p_u} \right)^{1/2} \left\{ \frac{2 \gamma}{\gamma - 1} \left[ 1 - \left( \frac{p_d}{p_u} \right)^{(\gamma - 1)/\gamma} \right] \right\}^{1/2} \]  

(7.20)

where \( R \) is ideal gas constant and \( \gamma \) is heat capacity ratio. When flow is choked, which is a condition defined by Equation(7.21), the mass flow rate through the valve is written as the form given in Equation(7.22).
\[
\frac{p_d}{p_u} \leq \left(\frac{2}{\gamma + 1}\right)^{\gamma/(\gamma-1)} \tag{7.21}
\]

\[
\dot{m} = \frac{C_d A_R p_d}{(R T_u)^{1/2}} \gamma^{1/2} \left(\frac{2}{\gamma + 1}\right)^{(\gamma+1)/2(\gamma-1)} \tag{7.22}
\]

Definition of the discharge coefficient \(C_d\) and selection of reference geometric flow area \(A_R\) are linked together. The product of these two terms is the effective flow area of the valve. This work uses a nominal geometric area defined by Equation (7.23) as a reference. Therefore, the experimentally measured discharge coefficient, \(C_d\), lumps together changes due to variations of both the cross-sectional area and flow effects.

\[
A_R = \frac{\pi}{4} D_{\text{valve}}^2 \tag{7.23}
\]

**Two-pressure Model**

Orifice flow equations are widely used in simulations to predict mass flow across the valves. To implement these equations, gas pressures upstream and downstream of the valve need to be known. In real-world engine applications, these two pressures need to be either measured or modeled. The first option is to measure both pressures; in this work we call this approach the ‘Two-pressure’ model. Gas pressure measurements in the vicinity of the valve will include all the possible effects resulting from the upstream dynamics, turbocharging, EGR and air-fuel mixing. As long as the measurements on both the runner side and in-cylinder are accurate (ideal condition), application of the
compressible flow equation is a universal solution which can be directly implemented in various engine platforms.

However, several challenges are associated with direct measurements of intake and cylinder pressures. The first and the foremost challenge is the added cost. Additionally, the calculation of mass air flow rate is crank-angle based, so it requires suitable pressure transducers and data acquisition systems capable of very high sampling rates. This would add significant cost to a production system. The second challenge is the implementation of pressure transducers. The pressure measurements need to be taken at the vicinity of the intake valve. For the upstream side, since pressure gradients exist in the intake port, the further the sensor is located from the valve, the higher the measurement error. The packaging of the cylinder head is already tight, so adding pressure transducers very close to the valve seat creates a substantial design challenge. The third challenge is signal-to-noise ratio of the cylinder pressure transducer. The transducer would presumably be used for both intake charge estimation and combustion diagnostics. In that case the sensitivity at near-ambient pressure level may be low, thus amplifying the noise and possible drift on a relative basis. Figure 7.4 shows the effect of slight measurement error on the prediction of mass flow rate. A 1% error in intake runner pressure measurement causes a very significant drift in the calculated mass flow rate away from the baseline.
Figure 7.4. Effect of pressure Measurement Error on mass flow rate calculation.

Single-pressure Model

Given the aforementioned challenges associated with the sensitivity of the Two-pressure model based on direct pressure measurements, it is necessary to investigate other methods of implementing orifice equations for air charge mass-flow prediction. The key contribution of this work is the development of an approach that simultaneously predicts one of the pressures and the mass-flow rate, and requires measurements of pressure on only one side of the valve.

The new approach is termed a “Single-pressure” model. Firstly, it eliminates the need for cylinder pressure measurement, and relies only on availability of crank-angle resolved gas pressure values in the intake port, just upstream of the valve. Secondly, to facilitate real-world implementation, we propose measurements of intake pressure profiles offline, and storing them in ECU memory as a lookup table. Formulation of the
model is presented first, followed by the discussion of the extension that allows real-world implementation using only a MAP signal.

The *Single-pressure* mass-flow prediction algorithm is a combination of orifice and continuity equations. Looking at the cylinder as the control volume, the dynamics of gas mass \( m_{cyl} \) variations in the cylinder as a function of cylinder volume \( V_{cyl} \) and gas density \( \rho_{cyl} \) can be written as:

\[
m_{cyl} = V_{cyl} \rho_{cyl} \quad (7.24)
\]

\[
\dot{m}_{cyl} = \dot{V}_{cyl} \rho_{cyl} + V_{cyl} \dot{\rho}_{cyl} \quad (7.25)
\]

For isentropic flow, density of the gas can be reduced to a function of cylinder pressure and heat capacity ratio \( \gamma \). Gas density in the cylinder, and its first order derivative can be written as:

\[
\rho_{cyl} = C_\rho P_{cyl}^{1/\gamma} \quad (7.26)
\]

\[
\dot{\rho}_{cyl} = \frac{C_\rho}{\gamma} P_{cyl}^{-1} \dot{P}_{cyl} \quad (7.27)
\]

where \( C_\rho \) is density constant. Substitute Equation(7.26) into Equation(7.27) allows the derivative of cylinder gas density to be a function of cylinder gas density, pressure, pressure derivative and \( \gamma \):

\[
\dot{\rho}_{cyl} = \frac{\rho_{cyl} \dot{P}_{cyl}}{\gamma P_{cyl}} \quad (7.28)
\]

Substitute Equation(7.28) to Equation(7.25) eliminates the derivative term of cylinder gas density\( (\dot{\rho}_{cyl}) \). The cylinder mass flow rate, \( \dot{m}_{cyl} \), can now be written as a
function of cylinder gas density, \( \rho_{cyl} \), cylinder pressure, \( p_{cyl} \), and the derivative of cylinder pressure:

\[
\dot{m}_{cyl} = \dot{V}_{cyl} \rho_{cyl} + V_{cyl} \frac{\rho_{cyl} \dot{p}_{cyl}}{\gamma p_{cyl}}
\]  
(7.29)

Substitute Equation (7.26) into Equation (7.29) eliminates the density term. Thus, cylinder mass flow rate becomes a function of the density constant \( C_\rho \), cylinder pressure, cylinder volume and their first order derivatives, i.e.:

\[
\dot{m}_{cyl} = C_\rho p_{cyl} \gamma \left( \dot{V}_{cyl} + \frac{V_{cyl} \dot{p}_{cyl}}{\gamma p_{cyl}} \right)
\]  
(7.30)

Combining the ideal gas law shown in (7.19) and Equation (7.26) for the isentropic process yields an expression for the density constant, \( C_\rho \), as a function of reference pressure, \( p_0 \), and temperature, \( T_0 \):

\[
C_\rho = p_0^{\frac{1}{\gamma} \left( \frac{1}{\gamma} - 1 \right)} \cdot \frac{1}{RT_0}
\]  
(7.31)

In this work, a two-stage isentropic assumption was established: one for the valve overlap stage, and another for the non-overlap stage. During valve overlap, residual gas is hot and some exhaust gas flows back into the cylinder. The cylinder gas temperature during this stage is close to the exhaust temperature. During the non-overlap stage, fresh air-fuel mixture flows into the cylinder and cylinder gas properties are dominated by intake gas. The density constant is calculated accordingly, i.e.:

- During the overlap stage, reference pressure \( p_0 \) is the exhaust back pressure and reference temperature \( T_0 \) is the exhaust temperature.
During the non-overlap stage: reference pressure $p_0$ is MAP and reference temperature $T_0$ is the intake temperature in the manifold.

Now consider that two equations for the mass-flow rate in or out of the cylinder have been derived, namely Equation (7.30) and Equation (7.20) or (7.22). Consequently, Equation (7.30) can be combined with orifice Equations (7.20)-(7.22), while postulating that cylinder mass flow rate is equal to the sum of flow rates across the intake and exhaust valves. For engines with four valves per cylinder, the output from the orifice equations need to be multiplied by two to arrive at total intake or exhaust flow. The combined state equation can now be written as:

$$
\sum (\dot{m}_{\text{intake}} + \dot{m}_{\text{exhaust}}) = C_{\rho} p_{\text{cyl}} \left( \dot{V}_{\text{cyl}} + \frac{V_{\text{cyl}} \dot{p}_{\text{cyl}}}{\gamma p_{\text{cyl}}} \right)
$$

(7.32)

This equation couples the cylinder mass flow rate and mass flow rate through the valves. It takes into account the effect of cylinder volume variation ($\dot{V}_{\text{cyl}}$), which is a function of cylinder geometry and engine speed. Therefore, cylinder pressure and its first order derivative are the only unknown parameters on the right hand side. Equation (7.32) can be written as a differential equation of cylinder pressure:

$$
\dot{p}_{\text{cyl}} = \frac{\dot{m}_{\text{cyl}} \gamma}{C_{\rho} p_{\text{cyl}} \frac{1}{\gamma - 1} V_{\text{cyl}}} - \frac{\dot{V}_{\text{cyl}} \gamma p_{\text{cyl}}}{V_{\text{cyl}}}
$$

(7.33)

Solving the ordinary differential equations (ODE) in Equation(7.33), and Equations (7.20)-(7.22) provide both charge mass and cylinder pressure value at every calculation step.
Figure 7.5 gives a summary of the “Single-pressure” algorithm for air mass flow rate estimation based on crank-angle resolved intake port pressure. The valve mass flow modules estimate the flow through the valves using the orifice equations. The sum of intake and exhaust valve flow is fed into the cylinder pressure calculation module, where Equation (7.33) is integrated at each time step to obtain the instantaneous value of cylinder pressure. The calculated cylinder pressure is subsequently fed into flow calculation modules to determine mass flow rate through both valves. Finally, the mass flow rate through the intake valve is integrated to yield total mass of intake charge.

\[ \dot{m}_{\text{intake}} = \int \dot{m}_{\text{in}} \, dt \]

Figure 7.5. Schematic diagram of pressure prediction and flow calculation scheme for the Single-pressure model.

The flow prediction algorithm calculates mass flow across the valves, where the composition of gas is a combination of air, fuel and EGR for port fuel injection (PFI) engines or air and EGR for direct injection (DI) engines. The total mass entering each cylinder in one engine cycle, \( \bar{m}_{\text{total}} \), is the sum of all components:

\[ \bar{m}_{\text{total}} = \bar{m}_{\text{EGR}} + \bar{m}_{\text{air}} + \bar{m}_{\text{fuel}} \]  (7.34)
For engines with EGR, the EGR mass fraction $x_{EGR}$ is defined as the mass of EGR divided by the sum of air and EGR masses, as given in Equation (7.35). For engines with port fuel injection, air and fuel are mixed before reaching the intake valve. Therefore, mass of fuel can be represented as a function of air mass $m_{air}$ and air-fuel equivalence ratio $\lambda$, as given in Equation (7.36).

$$x_{EGR} = \frac{m_{EGR}}{m_{air} + m_{EGR}} \quad (7.35)$$

$$m_{fuel} = \frac{m_{air}}{14.7\lambda} \quad (7.36)$$

In a multi-cylinder engine, the total air mass flow rate, $\dot{m}_{air}$, can be written as a function of mass of air entering each cylinder per cycle, $m_{air}^{cyl}$, number of cylinders, $n_{cyl}$, and engine speed:

$$\dot{m}_{air} = m_{air}^{cyl} \cdot n_{cyl} \cdot RPM \cdot \frac{1}{120} \quad (7.37)$$

Substitute Equations (7.35) and (7.36) into (7.34), the air mass per cycle $m_{air}^{cyl}$ can be written as a function of total mass $m_{total}$, EGR mass fraction $x_{EGR}$ and $\lambda$:

$$m_{air}^{cyl} = \frac{14.7\lambda(1-x_{EGR})}{1-x_{EGR} + 14.7\lambda} m_{total} \quad (7.38)$$

By substituting Equation (7.38) into (7.37), the mass air flow through the intake valve can be written as a function of the predicted total charge mass per cylinder per cycle, $m_{total}$, as shown in Equation (7.39). For engines with direct injection, only air and EGR are present in the intake system, thus the equivalence air fuel ratio $\lambda$ at intake becomes infinity. Equation (7.39) will transform to Equation (7.40).
\[
\dot{m}_{\text{air}} = \frac{14.7 \lambda (1 - x_{\text{EGR}})}{1 - x_{\text{EGR}} + 14.7 \lambda} \bar{m}_{\text{total}} \cdot n_{\text{cyl}} \cdot \text{RPM} \cdot \frac{1}{120}
\]  

\[
\dot{m}_{\text{air}} = (1 - x_{\text{EGR}}) \bar{m}_{\text{total}} \cdot n_{\text{cyl}} \cdot \text{RPM} \cdot \frac{1}{120}
\]  

**Intake Runner Pressure Lookup Model**

The air charge prediction algorithm requires crank-angle resolved intake runner pressure as model input. The most straightforward solution is to install a pressure transducer at intake runner. However, pressure transducers are generally very expensive. Additionally, the space at cylinder head are already limited, and adding a pressure transducer at the runner close to the intake valve will further complicate cylinder head design. Moreover, the intake pressure signal needs to have crank-angle or at least near crank-angle resolution, which is demanding on the data acquisition storage systems. Hence using a pressure transducer to provide input to the model is not likely to be the solution for production cars.

Instead of directly measuring the intake runner pressure, the pressure profile at the intake runner can be modeled. Numerical methods to model the intake gas dynamics have been extensively studied in published work[146-148]. However, these numerical solutions require to grid the intake manifold and runner into multiple elements and solve them individually, which requires significant amount of computing power and is not an optimal solution for real-time applications.

Another possible solution is to measure the intake runner pressure profile offline and store them as a look-up table. As shown in Figure 7.6, for the same intake and
exhaust valve timings, the intake runner pressure profile is largely a function of engine speed, while the load does not alter the basic profile of intake pressure much, which makes the look-up approach simple and reliable. Another observation can be seen from this figure is that intake runner gas dynamics varies greatly with engine speed, and the gas dynamics do not follow a sinewave or other simple waveform. Instead, wave action is a combined effect of intake runner design, valve actuation and engine rotational speed. A simple spring-damper modeling approach will not generate enough fidelity while a detailed model will take too much of computing effort.

Figure 7.6 Intake runner pressure dynamics vs. engine speed and load

The intake runner pressure look-up model used in this work stores information of pressure dynamics at the runner and to be used as input for the air charge prediction
model. Instead of storing the absolute pressure, the pressure difference between the runner pressure and MAP is stored:

\[ \Delta P = P_{\text{runner}} - MAP \]  \hspace{1cm} (7.41)

where \( P_{\text{runner}} \) is the crank-angle resolved runner pressure measured from experiments and MAP is from the measurement of the MAP sensor, which remains as constant at each engine cycle. In real time applications, the pressure information from the MAP sensor together with engine speed are used as inputs for the pressure look-up model. Using the pressure difference instead of absolute intake pressure allows usage of MAP sensor as direct input and makes interpolation between load points more reliable. In this work, 24 experiment data sets gridded with 8 engine speeds and 3 engine loads were used to generate a 3-D intake pressure lookup table. The data stored in this lookup table is shown in Figure 7.7.

![Figure 7.7 Intake runner pressure lookup table data as a function of engine speed, load and crank angle](image)

Figure 7.7 Intake runner pressure lookup table data as a function of engine speed, load and crank angle
For engines with variable valve timing, another degree of freedom is presented to the intake lookup model. As observed from experimental tests, valve timing will affect the phasing of the intake runner gas dynamics while its effect on the pressure profile is minimal. In this work, intake valve profile (ICL) and exhaust valve profile centerline (ECL) are used to represent the timing of intake and exhaust valves. It was observed from experimental studies that ICL only affects the phasing of intake runner pressure wave while effect from ECL is minimal. Based on this observation, the intake pressure lookup model can be modified to include ICL as an additional input. It was also observed that the change of ICL displays a linear correlation to the phase shift of intake runner pressure dynamics. This correlation is simplified to:

\[ CA = \frac{(ICL_0 - ICL)}{2} + CA_{\text{lookup}} \]

(7.42)

where \( CA \) is the shifted crank angle array which includes the offset in phasing related with ICL, \( ICL_0 \) is the reference position of intake cam phasing which is the same as the ICL used when collecting the experiment data and \( CA_{\text{lookup}} \) is the crank angle array for the pressure data in the lookup table. Figure 7.8 shows an example of using the intake runner pressure lookup model to incorporate the effect of varying ICL. Figure 7.8(a) shows the relation between runner pressure dynamics and ICL. It is shown that when intake valve timing advances (reduced ICL value), the runner pressure profile shifts to the left, while its profile changes slightly and maintains the same frequency and amplitude characteristics. Figure 7.8(b) shows the output from the intake runner pressure lookup table. The pressure profiles were taken experimentally when ICL is fixed at 128deg.
ATDC. The pressure profiles at other cam timing positions are obtained from the algorithm given in Equation (7.42). To further evaluate the intake runner pressure lookup model, Figure 7.8(c) and (d) show comparison between intake runner pressure lookup model outputs and experimental data, where Figure 7.8(c) shows the advanced timing condition (ICL = 113deg ATDC) and Figure 7.8(d) shows the retarded timing condition (ICL = 128deg ATDC). It is shown from Figure 7.8(c) that the intake pressure profile from the model well represents the experimentally measured pressure, especially the phasing and amplitude characteristics. As ICL moves away from the baseline (ICL = 128deg ATDC), the intake runner pressure lookup model starts to lose details on the intake pressure profile. This error is acceptable since it will be shown that the algorithm is robust with respect to intake pressure errors.
Figure 7.8 Intake runner pressure lookup model vs. experimentally measured runner pressure at various ICL positions

A schematic description for applying this intake runner pressure lookup model in a Simulink environment is given in Figure 7.9. The intake pressure profiles are stored as a 3-D lookup table with three inputs being crank angle, engine speed and MAP. The crank angle inputs are phased using the correlation given in Equation (7.42). In real-time applications, the table data is interpolated based on engine operating conditions including engine speed and load (MAP), as well as the number of times model iterates in each cycle which determines the input of CA.
Analysis and Results of VVT Applications

Simulation Validation

The air mass flow estimation model was first validated with GT-Power simulations. GT-Power is widely accepted as a reference 0-D/1-D engine simulation tool by both industry and academia. A virtual engine system was created by configuring the simulation to represent a V-6 engine, and providing key engine geometry information as input. Once the simulation is fully setup, it can provide valuable insights by generating outputs that cannot be easily measured in the test cell [96]. In this work, gas properties and valve flow characteristics are of primary interests, both of which are hard to measure in the running engine. The engine modeled in this study is based on a 3.6L V6. It is a naturally aspirated engine with variable valve timing and cooled EGR. Its specifications are given in Table 7.1.

Table 7.1. Specifications of the modeled Pentastar 3.6L V6 engine.
The intake and exhaust geometries and valve lift profiles have been carefully measured and supplied to the model. Accurate shape and volume data of the intake and exhaust manifolds is crucial for yielding satisfactory results, because gas dynamics play a key role in intake pressure-based charge estimation. The intake and exhaust discharge coefficients were determined experimentally using a flow rig. Figure 7.10 shows a comparison of simulated and experimental intake pressure dynamics in the intake runner, close to the manifold flange. In this case the engine is operated at 3000 rpm with manifold air pressure of 0.8 bar. The model is clearly capable of capturing the intake gas pressure dynamics with excellent accuracy. Similar agreements were achieved at other speed/load points.
Validation of the Two-pressure Model

The first step in the validation process was to examine the behavior of the **Two-pressure** model. The model was implemented in the Matlab/Simulink environment, and setup to span the period from intake valve opening (IVO) to intake valve closing (IVC). A fixed-step ODE solver was used for integration. The inputs and outputs of the **Two-pressure** charge mass estimation model are given in Table 7.2. Inputs in the left column are from GT-Power simulation.

Table 7.2. Inputs and outputs of Two-pressure charge estimation model for simulation validation.

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crank-angle resolved intake pressure</td>
<td>Intake valve total mass flow rate</td>
</tr>
<tr>
<td>Crank-angle resolved cylinder pressure</td>
<td>Total cylinder charged mass</td>
</tr>
<tr>
<td>Intake/Exhaust discharge coefficients</td>
<td>Total air mass flow rate</td>
</tr>
</tbody>
</table>
Cylinder volume
Intake/exhaust temperature
Exhaust back pressure
EGR percentage
Lambda

Figure 7.11 illustrates validation of the *Two-pressure* model using the GT-Power simulation data as a reference. In this case, Equations (7.20)-(7.22) are used to calculate the flow through the intake valve. The ideal gas constant, \( R \), is \( 287 \, \text{J/kg-K} \) and heat capacity ratio, \( \gamma \), is a constant 1.4. It is observed that the *Two-pressure model* with constant \( R \) and \( \gamma \) yields very good agreement with the GT-Power simulation in terms of mass flow rate through the intake valve, as long as accurate intake and cylinder pressure are used.

Figure 7.11. Validation of Two-pressure flow prediction model with GT-Power simulation data.
To investigate the robustness of the *Two-pressure* model, a sensitivity analysis was conducted with respect to model inputs. As mentioned at the beginning, the *Two-pressure model* is very sensitive to pressure inputs. Gas properties are also an important factor. Figure 7.12(a) shows model sensitivity with respect to variations of $\gamma$ and Figure 7.12(b) shows its sensitivity to intake pressure. The baseline condition is established with the *Two-pressure* model with results generated using $\gamma = 1.4$ and GT-Power simulated intake pressure as inputs. A summary of sensitivity analysis is given in Figure 7.13, where the effects of input errors on the final charge estimation results are quantified. It can be seen from Figures 7 and 8 that the *Two-pressure* algorithm demonstrates:

- Minimal sensitivity to $\gamma$, thus the usage of a detailed gas property model is not necessary. A constant $\gamma$ value would yield prediction results very close to those using a $\gamma$ calculated in real-time, with significantly reduced computational effort.
- There is a proportional relationship between the model error and the discharge coefficient.
- Relatively small effect of the intake gas temperature on prediction results.
- Extreme sensitivity to intake pressure errors. With only a 1% drift in intake pressure, the predicted intake charge mass can be off by more than 70%. Thus, a highly accurate and well filtered intake pressure signal is paramount for achieving high fidelity of predictions.
Figure 7.12. Model sensitivity to Gamma and intake pressure.
Validation of the Single-pressure Model

The Two-pressure model study has shown that model produces excellent results when accurate intake pressure and discharge coefficient inputs are used. However, extreme sensitivity to pressure profiles provided as inputs makes it unsuitable for practical applications. In the effort to solve this, the Single-pressure approach was developed. As shown in Figure 4, only intake pressure is used as an input and cylinder pressure is calculated simultaneously with the mass flow rate. The inputs and outputs of the Single-pressure charge estimation model are given in Table 7.3. They are similar to Table 7.2 but in the case of the Single-pressure model crank-angle resolved cylinder pressure is no longer a model input.
Table 7.3. Inputs and outputs of Single-pressure charge estimation model.

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crank-angle resolved intake pressure</td>
<td>Intake valve mass flow rate</td>
</tr>
<tr>
<td>Intake/Exhaust discharge coefficient</td>
<td>Total cylinder charged mass</td>
</tr>
<tr>
<td>Cylinder volume</td>
<td>Total air mass flow rate</td>
</tr>
<tr>
<td>Intake/exhaust temperature</td>
<td></td>
</tr>
<tr>
<td>Exhaust back pressure</td>
<td></td>
</tr>
<tr>
<td>EGR percentage</td>
<td></td>
</tr>
<tr>
<td>Lambda</td>
<td></td>
</tr>
</tbody>
</table>

The Single-pressure model has the ability to calculate cylinder pressure based on intake/exhaust mass flow rates and engine operation conditions using simple inputs. Figure 7.14 shows that the cylinder pressure profile calculated using the Single-pressure algorithm agrees well with the GT-Power baseline. Similar to what was described in the section above, $\gamma$ has a constant value of 1.4 and $R$ of 287 J/kg-K. Therefore, the model provides an alternative way to find cylinder pressure, which eliminates the need to install a cylinder pressure transducer. Additionally, since constant values can be used for $\gamma$ and $R$, a detailed gas property model is not necessary, hence making the model robust and more computational efficient.
Figure 7.14. Cylinder pressure prediction by the Single-pressure model compared to GT-Power results.

A key advantage of the *Single-pressure* model compared to the *Two-pressure* model is robustness, i.e. a reduced sensitivity to intake pressure error. Since the *Single-pressure* model calculates cylinder pressure as a function of intake pressure, simultaneously with the mass flow rate, the error in intake pressure will be reflected in the calculated cylinder pressure. In other words, the algorithm includes an inherent self-compensating feature, thus making the prediction much more robust.

Figure 7.15(a) shows a condition where measured intake pressure has drifted 0.01 bar above its actual value. In the case of the *Single-pressure* model, cylinder pressure is no longer from measurements; rather, it is calculated from the intake pressure by simultaneously solving differential equations for the cylinder pressure and mass flow rate. Figure 7.15(a) shows that calculated cylinder pressure reflects the intake pressure error and hence is slightly higher than the actual cylinder pressure. However, the air mass flow rate prediction shown in Figure 7.15(b) is very accurate, since the cylinder pressure...
adapted to the error of intake pressure. This confirms the self-compensating feature of the algorithm. In contrast, the Two-pressure model results shown in Fig. 10(b) are demonstrate very large errors in both the profile of the crank-angle resolved signal and the final cumulative mass. The Single-pressure model’s sensitivity to pressure inputs is greatly reduced, and it is much more robust compared to the Two-pressure model.

![Figure 7.15. Comparison between Two-pressure and Single-pressure model in terms of intake air flow rate prediction when intake pressure is drifted.](image)

The Single-pressure model was further validated with GT-Power simulation by carrying out multiple operating condition sweeps, including speed, load, cam timing,
EGR and ambient temperature. The goal was to test the robustness of the model over a range of steady-state engine operation conditions. Transient performance will be discussed in a later section. Total mass of charge per engine cycle was used to evaluate model accuracy. Table 7.4 gives a detailed summary of prediction error range for each actuator sweep. Figure 7.16 shows a detailed comparison between model-predicted total charged mass per cycle and the GT-Power simulation, the latter effectively serving as the “virtual engine”. Model error is less than 1.2% in all tested cases.

Table 7.4. Single-pressure model validation with GT-Power actuator sweeps: Tested items and model error.

<table>
<thead>
<tr>
<th>Actuator</th>
<th>Tested cases</th>
<th>Absolute error range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load sweep</td>
<td>2000/4000rpm, 0.2~0.9bar MAP</td>
<td>0.08~1.18%</td>
</tr>
<tr>
<td>Speed sweep</td>
<td>0.5/0.8bar MAP, 1000~4500rpm</td>
<td>0.16~1.10%</td>
</tr>
<tr>
<td>Cam timing sweep</td>
<td>3000rpm, 0.8bar MAP, ICL ± 10 deg, ECL ± 10 deg</td>
<td>0.09~1.07%</td>
</tr>
<tr>
<td>EGR sweep</td>
<td>3000rpm, 0.8bar MAP, EGR percentage 0%~20%</td>
<td>0.12~1.17%</td>
</tr>
<tr>
<td>Ambient temp sweep</td>
<td>3000rpm, 0.8bar MAP, Ambient Temperature -30~40℃</td>
<td>0.35~0.54%</td>
</tr>
</tbody>
</table>
Figure 7.16. Single-pressure model validation with GT-Power actuator sweeps. (a): speed and load sweep; (b): EGR, ambient temperature and cam timing sweep.

Experiment Validation of the Single-pressure Method
The physics based *Single-pressure* air charge mass prediction model was further validated with experimental tests. An environmentally controlled 430kW engine dynamometer test cell was used for the experimental study – see Figure 7.17. The engine was a naturally-aspirated 3.6L V-6 port fuel injected spark-ignited engine, equipped with hydraulically-driven dual-independent cam phasing on both banks. The specifications of this engine are given in Table 7.1.

![Figure 7.17. Schematic diagram of experimental test setup. The photo is showing the 430 kW transient AC dynamometer test cell with Chrysler 3.6L V6 Pentastar engine.](image)

The data acquisition system was a 32 channel system with capability of sampling in a 0.25 crank-angle degree interval. AVL GH12D piezoelectric pressure transducers were used to measure cylinder pressure and Piezoresistive Kulite sensors were used for both intake and exhaust pressure measurements. The exhaust pressure sensors were mounted on the exhaust manifold and water-cooled to minimize signal drift. Thermocouples were installed in both the intake and the exhaust manifold. Two Bosch LSU 4.9 wide-band lambda sensors were installed pre- and post-catalyst in addition to
stock lambda sensors. AVL Indicom was used to record cycle-by-cycle signals. An ETAS INTECRIOS system was used to override the stock engine control system when needed.

**Steady-state Validation**

The model was first validated under steady-state engine operating conditions, where all engine actuators were fixed at each test point. The *Two-pressure* and *Single-pressure* models were validated with experimental data and a comparison was made between the prediction results of the two algorithms. Table 7.5 gives model inputs for offline validation. The intake temperature used in this model was from the stock engine ECU. Exhaust temperature was also from a temperature model built in the stock ECU.

Table 7.5. Inputs of off-line model validation based on experiment data.

| Experimental measurement | Crank-angle resolved intake pressure  
|                          | Crank-angle resolved cylinder pressure*  
|                          | Intake/exhaust temperature  
|                          | Engine speed  
|                          | Manifold air pressure  
|                          | Cam timing (ICL, ECL)  
|                          | Lambda  
|                          | EGR percentage  
| Engine geometrical data | Cylinder and cranktrain geometry  
|                          | Valve discharge coefficients  
|                          | Valve lift profile  
| Constants               | Ideal gas constant R  
|                          | Hear capacity ratio $\gamma$  


Exhaust back pressure (1 bar)
* Cylinder pressure is only used as input in Two-pressure model.

Figure 7.18 shows steady-state validation results using both the Two-pressure and Single-pressure models offline. Figure 7.18(a) shows measured intake pressure, cylinder pressure and modeled cylinder pressure using the Single-pressure algorithm. The engine speed in this case was 3000rpm and MAP was 0.8 bar. It can be seen that cylinder pressure exceeds intake pressure between 100 to 200 crank angle degrees ATDC. This is likely due to cylinder pressure measurement error, since cylinder pressure higher than intake pressure would cause a gas backflow, which is not likely during the middle of the intake stroke. Cylinder pressure was referenced with intake pressure, thus a drift of cylinder pressure compared to its absolute value may exist. The range of cylinder pressure transducers used in this study is up to 200 bar, and the accuracy at pressures close to 1 bar deteriorates. These factors combined lead to a large estimation error in case of the Two-pressure method.

Figure 7.18(b) shows a comparison of the total charge mass per cycle predicted using the Two-pressure and Single-pressure models. The predictions generated with the Two-pressure model are completely unrealistic, since the final value of fresh charge mass is negative. The erroneous positive pressure differential between the cylinder and the intake port led to unrealistically high back flow prediction. In contrast, the Single-pressure model achieved acceptable accuracy, with the predicted total intake charge mass very close to the target value - see Figure 7.18(b). This was in part due to the self-
correcting feature of the *Single-pressure* algorithm, stemming from the fact that the cylinder pressure is calculated by simultaneously solving ODEs for cylinder pressure and mass flow. In short, the *Single-pressure* algorithm is capable of robust performance due to both (i) the elimination of error-prone cylinder pressure measurements during gas exchange, and (ii) the ability to compensate for any error in the intake pressure measurement.

Figure 7.18. Comparison of flow prediction model validation with experiment data between Two-pressure and Single-pressure method.
As has been shown in Figure 7.5, cylinder pressure is obtained by integrating the ODE in Equation (7.33). This requires knowledge of initial cylinder pressure to start the calculation. In the validation exercise presented in the previous section, initial cylinder pressure was set to match the GT-Power predicted cylinder pressure at IVO. In real world applications, it is difficult to accurately measure the cylinder pressure at IVO; in addition, a goal of this research is to avoid the need for installing cylinder pressure transducers. Therefore, constant initial cylinder pressure at IVO is used for all Single-pressure calculations across the range of engine conditions. The results confirm the ability of the Single-pressure model to compensate for the initial error of cylinder pressure and converge on the correct value in a small number of iterations. A drift of initial cylinder pressure will affect the calculation of intake and exhaust mass flow, which in turn counteracts the error of cylinder pressure. For instance, when initial cylinder pressure is lower than the true value, the calculated intake mass flow rate will be lower than the true value due to the reduced pressure difference, causing cylinder pressure to decrease slower and then converge to the true value. Figure 7.19 illustrates the process described above, by comparing the Matlab/Simulink estimation results to the GT-Power baseline. It is shown that the calculated cylinder pressure converges to its true value over a period of only few degrees CA.
Figure 7.19. Demonstration of cylinder pressure prediction converged to true value where initial error was present.

The validation process is extended to include comparisons of Single-pressure predictions and experiments for multiple engine actuator sweeps. In this section, mass air flow rate determined by the ECU was used for validation, and only the Single-pressure model was evaluated. The ECU mass air flow model is based on the speed density approach with an extensively calibrated volumetric efficiency function. The objective was to obtain $\leq 5\%$ error with the Single-pressure charge estimation model compared to ECU baseline.

Figure 7.20 shows the validation of estimated values for engine speed and load sweeps. Engine speed varied from 1000 to 4500 rpm, with manifold air pressure of 0.3 bar, 0.5 bar and 0.8 bar for each engine speed. The root-mean-square error (RMSE) was used to evaluate model prediction accuracy, as defined in Equation (7.43), where $n$ is the total number of points, and $\dot{m}$ and $\hat{m}$ are experimentally measured and model predicted
air mass flow rates, respectively. The *Single-pressure* model is clearly able to accurately predict steady-state mass flow rates across the range of engine speed-load conditions. As shown in Figure 7.20(b), model prediction errors are within a 3% error band, with RMSE of 0.74 g/s.

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{m}_i - \bar{m}_i)^2}{n}} \tag{7.43}
\]
Figure 7.20. Results of Single-pressure model validated with steady-state experiment data.

The model was also validated with experimental actuator sweeps. Commands were varied for one actuator at a time, with all other actuators fixed. For instance, when an EGR sweep was conducted, engine speed, load, cam timing and spark timing were held at constant values to eliminate disturbances from other factors. Figure 7.21 shows model validation results with EGR, lambda and cam timing sweeps. Test conditions and mass-flow rate model prediction errors are summarized in Table 7.6. The Single-pressure model demonstrated a sufficient degree of fidelity and captured the change of engine cam timing, air fuel ratio and EGR levels with errors below 3.2%.

Table 7.6. Model validation with experimental actuator sweeps: Tested items and model error.
<table>
<thead>
<tr>
<th>Actuator</th>
<th>Tested cases</th>
<th>Absolute error range</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICL sweep</td>
<td>3000rpm, 0.8bar MAP, ICL = 113~128deg</td>
<td>0.87~1.63%</td>
</tr>
<tr>
<td>ECL sweep</td>
<td>3000rpm, 0.8bar MAP, ECL = 102~114deg</td>
<td>0.23~0.68%</td>
</tr>
<tr>
<td>EGR sweep</td>
<td>2000/3000rpm, 0.5/0.8bar MAP, EGR percentage 5%~15%</td>
<td>0.32~3.22%</td>
</tr>
<tr>
<td>Lambda sweep</td>
<td>2000rpm, 0.5bar MAP, $\lambda = 0.8$~1.2</td>
<td>1.80~1.92%</td>
</tr>
</tbody>
</table>

Figure 7.21. Results of Single-pressure model validated with steady-state experiment data. Including EGR, lambda and cam timing sweeps.

Real-Time implementation and Online Transient Validation

The ultimate goal of this work is to develop a physics based intake charge estimation algorithm which is capable of in vehicle real-time implementation. This
demands the model yield good transient performance since engines in vehicles seldom operate at steady-state conditions. The fact that the proposed Single-pressure algorithm uses intake pressure as an input, and the latter has much faster dynamics than the upstream mass flow rate, makes it a promising approach.

To investigate the transient performance of the Single-pressure method, the Matlab/Simulink based model was converted to C and flashed into an ETAS ES910 ECU which runs real-time in parallel to the existing engine controller. The model inputs for real-time validation are given in Table 7.7. They are similar to the steady-state model inputs shown in Table 7.5, except for the fact that the measured intake pressure is now substituted with pre-stored lookup table. The lookup table contains the crank-angle resolved intake pressure profile for multiple engine speeds. For online applications, this table will be interpolated at various engine speeds.

Table 7.7. Inputs of online model validation.

<table>
<thead>
<tr>
<th></th>
<th>Intake/exhaust temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real-time measurement</td>
<td>Engine speed</td>
</tr>
<tr>
<td></td>
<td>Manifold air pressure</td>
</tr>
<tr>
<td></td>
<td>Cam timing (ICL, ECL)</td>
</tr>
<tr>
<td></td>
<td>EGR percentage</td>
</tr>
<tr>
<td>Pre-stored lookup table</td>
<td>Intake runner pressure</td>
</tr>
<tr>
<td>Engine geometrical data</td>
<td>Cylinder and cranktrain geometry</td>
</tr>
<tr>
<td></td>
<td>Valve discharge coefficients</td>
</tr>
<tr>
<td></td>
<td>Valve lift profile</td>
</tr>
<tr>
<td>Constants</td>
<td>Ideal gas constant R</td>
</tr>
</tbody>
</table>
The model was validated over the federal transient driving cycle FTP-75 using an engine-in-the-loop capability in the engine dynamometer test cell. Air-fuel ratio and cam timings are controlled by the ECU stock calibration; thus, operating conditions strongly resembled real-world operation. The stock 3.6L engine is not equipped with EGR. The intake gas temperature signal was taken from the ECU. Figure 7.22(a) shows the model predicted mass air-flow rate and ECU predicted mass air-flow rate, engine speed, load, AFR and intake gas temperature over an 80 second segment of the transient test. Predicted mass air flow rate follows the ECU output signal closely, even during heavy transient conditions. Figure 7.22(b) shows a scatter plot correlating model predicted and ECU estimated mass air flow rate. It illustrates the model’s ability to keep mass air flow rate predictions within 5% of ECU’s output most of the time. The RMSE of model prediction during this transient driving cycle test was 0.82 g/s. In summary, the Single-pressure model demonstrates good transient performance with low prediction error (<5% error) in both steady state and transient conditions.
Figure 7.22. Validation results of Single-pressure model under transient driving cycle test.
In-vehicle Validation

To test the real-time performance of the physics based air charge prediction model, the algorithm was real-time implemented in a vehicle and tested on a proving ground. The schematic description of on-vehicle implantation is given in Figure 7.23. The tested vehicle is a minivan with the same engine used in the steady state dynamometer testing. The engine was equipped with VVT and has no EGR. The air charge prediction model was again compiled into C and was stored in ETAS ES910. Model parameters can be real-time adjusted on PC through INCA. The PC communicates with ECU through ES910, which enables real-time control of engine actuators including cam phasing, air-fuel ratio etc.

Figure 7.23 On-vehicle experimental setup for the proving ground test

In real-time applications, model execution speed is a critical parameter. Achieving best prediction results with acceptable computing power requirement is a guide line for the model development. In this work, the ETAS ES910 is used as benchmark to test the
model execution speed. If the model is capable to run with ES910 at every cycle throughout the engine speed range, it is believed the model would have potential for future on-vehicle real-time applications.

In this model framework, the parameter that governs the model execution speed is the iteration number, which is defined as the number of times the valve mass flow and cylinder pressure are updated during the intake process per engine cycle. The iteration number determines the resolution and accuracy of the model. The higher the iteration number is, the better accuracy and more details of intake flow and cylinder pressure information can be acquired. However, higher iteration number requires more computation power. Thus a compromise need to be made between prediction accuracy and computing power requirement. Figure 7.24 shows the relationship between model prediction accuracy and iteration number (represented as N). The RMSE values are acquired from offline simulations with data recorded from the proving ground as input. It is shown that when iteration number is lower than 150, RMSE quickly increases and becomes unacceptable. On the other hand, as the iteration number is over 200, the improvement on model prediction accuracy becomes minimal. Based on this, an optimal number of 180 was selected to strike a balance between model prediction accuracy and computing power requirement. The model execution time with iteration number of 180 in ES910 environment is 0.013s, which allows the model to run every engine cycle with engine speed up to 9230rpm.
The vehicle driving profile during the real-time test incorporated constant speed cruising, hard acceleration and idle, which covers most of conditions in normal vehicle operation. Due to the safety limitation of the dynamometer facility, the intake runner pressure lookup data used in the air charge prediction model was tabulated with experimental data up to 4500rpm. To compensate the gap between 4500rpm to maximum engine speed (6500rpm), additional intake pressure profiles at higher engine speeds were offline generated from GT-Power simulation. Additionally, some engine speed dependent steady-state errors observed during the real-time test were believed to be associated with ill calibrated intake runner pressure lookup table. Small multipliers are applied to the intake profile at certain engine speeds to mitigate the speed dependent errors. Additionally, to avoid numerical issues, only interpolating is allowed in the intake runner pressure model while extrapolating outside the engine speed range was not allowed.
The mass air flow rate from ECU speed density model was used as baseline for validation in the real-time test. Figure 7.25 shows results of real-time online validation. The engine speed, load and cam phasing underwent heavy transients throughout the testing process. It is shown from the mass flow rate figure that the model tracks ECU predicted mass flow rate well and displayed good agreements during transients. The real-time test proves model’s ability to run real-time in ETAS ES910. Though the current generation of ECUs do not have the same level of computing power, model’s performance on ETAS system confirms its potential for future production car applications.
Since this air charge prediction model is feedforward only, once real-time performance is tested, the model can be further validated offline with recorded data. The model used in offline validation is the same as used in real-time applications with iteration number set to 180. Since real-time execution speed has been proven to work with entire engine speed range, the offline validation will have the same merit as compared to real-time validations.
To validate the intake charge prediction model comprehensively, a total number of four real-world driving data recorded from the proving ground were used for validation. These four cases incorporated normal city-like driving and occasional hard accelerations. Additionally, ambient air temperature and engine coolant temperature both varied during the four test cases, making the validation more comprehensive. Table 7.8 gives a summary of each driving profiles, including maximum engine speed reached, driving durations and mean intake air temperature. The RMSE of model predicted air mass flow compared to ECU baseline and percentage of time model prediction error is within 5% are also given for each test case. A direct comparison between model prediction and ECU baseline for all tested cases are shown in Figure 7.26. It is shown that at most of the time the model prediction error is within the 5% boundary.

<table>
<thead>
<tr>
<th></th>
<th>Case #1</th>
<th>Case #2</th>
<th>Case #3</th>
<th>Case #4</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE [g/s]</td>
<td>1.09</td>
<td>1.39</td>
<td>1.08</td>
<td>1.50</td>
</tr>
<tr>
<td>Time within 5% error</td>
<td>94.0%</td>
<td>94.9%</td>
<td>85.5%</td>
<td>95.6%</td>
</tr>
<tr>
<td>Max engine speed [RPM]</td>
<td>6496</td>
<td>6510</td>
<td>5006</td>
<td>5846</td>
</tr>
<tr>
<td>Mean intake air temp</td>
<td>304.5K</td>
<td>310.8K</td>
<td>316.6K</td>
<td>324.3K</td>
</tr>
<tr>
<td>Duration</td>
<td>330s</td>
<td>335.6s</td>
<td>125.7s</td>
<td>67.6s</td>
</tr>
</tbody>
</table>
It is shown from both steady state dynamometer and real-time proving ground validations that the physics based air charge prediction model developed in this work has the real-time running capability and generates accurate predictions of intake air mass flow in a naturally aspirated VVT engine. To demonstrate the fidelity of the model with respect to varying valve timings, Figure 7.27 shows a comparison of model prediction error as a function of valve overlap. Figure 7.27(a) shows the results when constant valve timing (in this case ICL=128, ECL=117) is used as model input, while in Figure 7.27(b) true positions of intake and exhaust cams are used as input. It is shown that the prediction accuracy greatly enhances when true cam positions are used as input. The model has
displayed its fidelity with respect to the valve timing, which results from the inherent
merit of physics based modeling approach.

Figure 7.27 Display of model fidelity on cam timings. (a) Prediction error with fixed cam
phasing as input; (b) Prediction error with true cam phasing as input
Simulation Study of VVA Applications

One of the objectives when developing the physics based air charge prediction model is to achieve cross-platform applications. Since the algorithm directly calculates flow rates at valves, ideally the same model structure should work with engines with varying valve profiles (VVA). In this work, the application of the proposed direct calculation method is evaluated on a Multiair engine. Due to the limited access to a production engine, only GT-Power validation was conducted. Although experimental data is not available, simulation studies are sufficient to test whether the same algorithm is applicable to Multiair engines and additionally, simulation studies help to provide insight to model developments.

Multiair engines are equipped with VVA systems, which enables control of not only valve timings, but also valve lift profiles. The exhaust cam in a Multiair engine is the same as the one used in a conventional VVT engine, i.e. only cam timing can be varied. The intake cam on the other hand, is connected with intake valve with a hydraulic chamber, which allows control of both timing and lift. Figure 7.28 shows an example of valve profiles in a Multiair engine. The exhaust lift is a fixed profile, while the intake lift profile can switch between multiple actuation modes. The hydraulic coupling between the intake cam and intake valves allows a Multiair engine to achieve two intake lift strategies: early intake valve closing (EIVC) and late intake valve opening (LIVO), which are both shown in Figure 7.28. Specifically, the EIVC strategy allows a long valve overlap period and enables a more flexible control of residual gas fraction (RGF) while LIVO strategy can be used for load control at part-load conditions. In this work, the
physics based air charge prediction is tested with full load, EIVC and LIVO strategies through simulation.

The model was validated with GT-Power simulations as baseline. The intake and exhaust geometries have been carefully measured and were used to configure the model. Accurate shape and volume data of the intake and exhaust manifolds is crucial for yielding satisfactory results because gas dynamics is the key for intake pressure based charge estimation. The intake and exhaust valve lift profiles and discharge coefficients were also experimentally determined.

The Multiair intake valve profile at full load, EIVC and LIVO conditions are validated with GT-Power simulations. The manifold air pressure for all conditions is set at 1 bar. Figure 7.29 shows the validation of full load condition. The tested condition is at engine speed of 3000rpm. The intake and exhaust lift profiles are also displayed in the figure for reference, where the numbers do not represent the true lift values. In the full load profile case, the intake profile and overlap characteristics are similar to that in a
conventional VVT engine, thus the same algorithm used for conventional engines also works well in this case. The model predicted cylinder pressure and intake valve air mass flow rate simultaneously with good accuracy.

Figure 7.29 GT-Power validation of air charge prediction model on a Multiair engine, full lift case
Figure 7.30 shows the validation results of EIVC intake strategy with the same air charge prediction model used in conventional VVT engines. The engine speed used in this test condition is 1000rpm. In EIVC conditions, it is clearly shown that a very long period of valve overlap is enabled by the boot-like intake valve profile during the initial stage of the intake event. It is shown that the cylinder pressure prediction during the overlap period and intake air mass flow rate prediction after TDC are drifted away from the true values. The error of cylinder pressure prediction during valve overlap period is due to constant exhaust pressure used as input in the modeling scheme. Constant exhaust pressure works well with conventional VVT engines where valve overlap period is considerably short and this approximation does not introduce significant error. In Multiair applications, EIVC strategies allow very long valve overlap (>100deg CA), where the flow at the exhaust valves plays a significant rule during the intake process; hence, constant exhaust pressure assumption does not hold. The intake air mass flow rate prediction error after TDC is also associated with the prolonged valve overlap period. This long overlap allows hot residual gas in the cylinder to flow back into the intake runner and alters the properties of intake gas.
Figure 7.30 GT-Power validation of air charge prediction model on a Multiair engine, EIVC case

Figure 7.31 shows the history of intake, exhaust and in-cylinder gas temperatures of the same case shown in Figure 7.30. The temperature profiles are from GT-Power.
simulation. It is shown that during the valve overlap period, intake temperature quickly increases to around 700K due to the backflow of hot in-cylinder residual gas. When fresh air starts to flow into the cylinder, the intake gas temperature quickly drops back to the same level as the air temperature before the intake runner. The intake air charge prediction model used for conventional VVT engines uses a constant as intake temperature input, thus the change in the intake gas property during the overlap period was not captured, resulted in prediction errors during the intake process.

![Figure 7.31 Illustration of intake, exhaust and cylinder gas temperature during the intake process at EIVC condition](image)

To address the two issues discovered in Figure 7.30, namely cylinder pressure prediction error during valve overlap and intake air flow rate prediction error, crank angle resolved exhaust pressure needs to be included as an additional input. In addition, an intake temperature model is required to predict the change in gas temperature during the
intake process. Therefore, a simplified plug-flow based intake temperature model is developed to estimate the change of intake temperature during the valve overlap period. As shown in Figure 7.32, during the intake process, mass transfer occurs between intake manifold and runner as well as between runner and cylinder. In the intake runner, gas flows from manifold and cylinder are assumed to be blended adiabatically, where no heat loss to the wall is allowed.

![Figure 7.32 Definition of control volume and boundary layers of the intake runner gas temperature model](image)

The gas temperature in the intake runner $T_{in}$ is calculated from the mass and temperature of gas from both boundary layers

$$T_{in} = \frac{m_1 T_1 + m_2 T_2}{m_1 + m_2} \tag{7.44}$$

where $m_1, T_1$ are the mass and temperature of the gas from intake manifold and $m_2, T_2$ are for the in-cylinder residual gas. Before the intake process starts, the gas in the intake runner share the same property as the intake manifold, where the mass in the intake
runner $m_{in}$ equals to $m_1$. The intake runner mass at the beginning of the intake stroke can be estimated as:

$$m_{in} = \frac{MAP \cdot V_{\text{runner}}}{RT_m}$$  \hspace{1cm} (7.45)

where $V_{\text{runner}}$ is the volume of the intake runner and $T_m$ is the manifold air temperature.

After intake valve opening, mass transfer starts to occur at both boundaries. If the direction of flow in the intake runner-cylinder boundary is from the cylinder to the runner, part of the mass in the intake runner will be displaced by the hot residual gas from the cylinder, and vice versa. The mass from the in-cylinder residual $m_2$ are obtained as an integral of mass flow rate through the intake valve $\dot{m}$. When the flow through the intake valve is going into the cylinder, $\dot{m}$ is positive and vice versa. Since the mass in the runner is partially displaced by the residual, the remaining mass of the gas from the intake manifold is determined as the difference between the initial runner mass $m_{in}$ and $m_2$, as defined in Equation(7.46). The lower bound of the numerical solution of either $m_1$ or $m_2$ is set to zero. When the bound is reached, it indicates no mass of this species exist in the runner.

$$m_2 = \int -\dot{m} dt \hspace{1cm} m_1 = m_{in} - m_2$$  \hspace{1cm} (7.46)

With inclusion of crank-angle resolved exhaust pressure profile and additional temperature model, the same case shown in Figure 7.30 is again validated with GT-Power. The validation results shown in Figure 7.33 clearly displays the improvement of model prediction accuracy in both the cylinder pressure and intake mass flow rate.
Figure 7.33 Improved model prediction accuracy with inclusion of intake runner gas temperature model and crank-angle resolved exhaust pressure information.

Similarly, the LIVO intake strategy is also validated with GT-Power simulations. Since the intake valve opens late in the intake stroke, very small or no valve overlap is
presented during the intake process, thus the effect from the exhaust side is negligible. Figure 7.34 shows the validation results of the LIVO valve strategy. Since the problem is reduced to intake flow – cylinder pressure only, the model is displaying good prediction results for both cylinder pressure and intake mass flow. However, the initial condition of cylinder pressure need to be specially addressed here. Due to the late opening of intake valve, the cylinder pressure at intake valve opening drops below the intake manifold pressure. Depend on the timing of intake valve opening, the initial cylinder pressure can be estimated as:

\[ p_{ini} = p_{ex} \left( \frac{V_0}{V_{IVO}} \right)^\gamma \]  

(7.47)

where \( p_{ex} \) is the exhaust backpressure, \( V_0 \) is cylinder clearance volume and \( V_{IVO} \) is the cylinder volume at intake valve opening. The heat capacity ratio \( \gamma \) is associated with the property of the residual gas which has similar property of exhaust gas, thus a constant value of 1.34 is assumed.
To further validate the application of intake air charge prediction model in a Multiair engine, GT-Power sweeps of engine speed for both EIVC and LIVO strategies are conducted to test the model performance. The total intake charge mass per cylinder
per cycle is used for validation. Figure 7.35 shows the validation results of speed sweeps for both EIVC and LIVO strategies. The charge mass predicted by the model shows good agreement with GT-Power simulation results at all engine speeds.

![Diagram showing validation results of speed sweeps for EIVC and LIVO strategies](image)

**Figure 7.35 Model validation results with GT-Power engine speed sweeps, EIVC and LIVO conditions**

From the simulation study, it is known that the air charge prediction algorithm developed for a VVT engine also applies for an engine with VVA. This cross-platform application potential is one of the inherent benefits of physics based models. However,
some parts of the algorithm need to be addressed specifically for VVA applications in comparison to VVT applications, namely: (i) at high overlap conditions, the intake temperature change due to excessive backflow need to be modeled to capture the change of intake gas property. (ii) for high overlap conditions, the gas exchange between cylinder and exhaust valves plays a more significant role in the intake process compared to conventional VVT engines, this would require more detailed information about the exhaust pressure dynamics.

There are some open question left with Multiair applications. First of all, this work only validates the model with simulation, additional experimental work is required to further test the performance of the model on VVA applications. Additionally, current model relies on offline measured intake pressure profile. For Multiair or other VVA engines, the change of valve profile would alter the characteristics of the intake runner pressure dynamics, adding one additional dimension to the table. The calibration effort of the lookup table can be further saved if physics based model of intake/exhaust pressure dynamics with moderate computing load can be developed.

**Conclusions**

In this work, a physics based crank-angle resolved intake charge prediction algorithm is proposed and validated. The model is based on 0-D modeling of the mass air flow at the intake valve. The novel aspect of the algorithm is its ability to provide robust simultaneous predictions of the crank-angle resolved flow through the valves and the estimate of the total mass of charge at IVC using intake pressure as a sole pressure input.
The system of differential equations derived in this work enables simultaneous prediction of charge mass flow and in-cylinder pressure, thus eliminating the need for expensive cylinder pressure measurements. Robustness of the algorithm stems from the (i) elimination of the need for in-cylinder pressure measurements which are error-prone at the low end of the range experienced during gas-exchange, and (ii) demonstrated low sensitivity to the error in intake pressure values. The latter is a consequence of the self-compensating features in the algorithm itself, i.e. ability of the algorithm to adapt the error in input thanks to the coupling of mass flow and pressure ODEs.

The first step in this effort was to develop and validate at Two-pressure method where both intake and cylinder pressure are measured and provided as input. Compressible flow equations are solved to determine the crank-angle resolved flow and ultimately integrate its value to estimate total mass. Results were validated using predictions obtained with a detailed 1-D GT-Power simulation. The Two-pressure model is very accurate if inputs are correct, but the sensitivity analysis revealed its high sensitivity to the error in the pressure measurement. This would be a problem in any real-world application due to difficulties in obtaining accurate low-pressure measurements with pressure transducers calibrated for a full range of cylinder pressure.

In contrast, the Single-pressure algorithm calculates cylinder pressure on a crank angle basis by updating a set of ODEs. It was first validated using the GT-Power simulation as a reference, followed by a detailed sensitivity analysis that demonstrated robustness with respect to both intake pressure input and the initial guess for cylinder pressure. Real-time implementation was subsequently evaluated through comparisons
with experimental measurements on a V6 SI engine in a research-grade test cell. The air charge prediction model was validated with steady state dynamometer testing, where speed, load and other actuator sweeps including lambda, cam timing and EGR sweep are conducted to test the performance and robustness at steady state. Actuator sweeps have proven the accuracy of the model at steady state regardless of engine operating conditions. Validation results prove the ability of the Single-pressure method to providing accurate prediction (within 5% error, in most cases <3%) of mass air flow in both steady state and transient conditions. The model also demonstrates fast transient response in the transient driving cycle test.

The model was subsequently tested on a proving ground where the algorithm was real-time implemented in a test vehicle. In both tests the model have displayed good prediction of intake air mass flow rate compared to the ECU baseline. Through the proving ground tests, an optimum iteration number of 180 was selected and the model was capable to run every cycle with engine speed up to 9230rpm. Additionally, the model have displayed good real-time performance even the engine is under heavy transients.

Simulation study to investigate the application of the air charge prediction model on a VVA engine is also conducted in this work. A GT-Power model of a Multiair VVA engine was used as baseline. The insights from the simulation study is that the air charge prediction algorithm developed for a VVT engine also applies for an engine with VVA, however, additional augmentations including an additional intake temperature model and more details about time-varying exhaust pressure are needed for valve strategies which enable long period of valve overlap.
Thanks to no additional sensor cost and robustness to inputs, the air charge prediction method has great potential for real-world engine applications. It is universally applicable, i.e. it has the potential to significantly reduce calibration effort for engines equipped with multiple actuators. The physics based air charge prediction model developed in this work also has the potential to be integrated with other physical models.

The scope of this work can be extended to the exhaust stroke to obtain crank-angle resolved information about exhaust flow. Therefore, both the cylinder pressure and flow through all valves during the gas exchange process can be estimated. This would provide a new way to estimate residual gas fraction in real-time. Since the output of this air charge prediction model provides initial conditions for a combustion model, and the combustion model generates the initial condition for the exhaust stroke, the combination of models would enable real-time engine cycle cylinder pressure prediction. This has great potential for future development of engine model predictive control.
CHAPTER EIGHT
CONTRIBUTIONS AND RECOMMENDATIONS FOR FUTURE WORK

This work has developed several physics-based models for enhancing predictiveness of engine system simulations, as well as providing accurate estimation for real-time control applications. The Quasi-D combustion model is developed in the context of a dual-fuel CI engine while a 0-D intake air charge prediction model is developed with SI gasoline engine applications in mind. The key contributions and recommendation for future work are summarized as follows.

Key Contributions

Quasi-D Dual-fuel Combustion Model

**Multi-zone diesel spray/combustion model for dual-fuel engine simulation**

1) Improved diesel spray tip penetration model. The spray penetration model in the existing spray-combustion simulations developed by Hiroyasu et al. fails to provide accurate prediction results due to the evolution of fuel injectors over the years. This work proposes an improved spray tip penetration algorithm based on the existing framework. The improved model was calibrated with experiments where modern high pressure, small hole diameter injector was used. The improved model displays good agreement with experimental data in both cases.
and shows considerable improvement compared to the existing Hiroyasu-Arai model.

2) Modified ignition delay correlation for diesel combustion with EGR. An ignition delay correlation for diesel combustion is developed in this work to accommodate the inclusion of EGR. The correlation is developed based on the work from Assanis et al., with oxygen concentration as an added parameter to account for the reduced oxygen concentration as a result from inclusion of EGR. The new correlation is developed with the aid of experimental data from a single cylinder research engine. The modified ignition delay correlation shows much better agreement with experimentally measured ignition delay at various operation conditions with varying level of EGR compared to the baseline ignition delay correlation.

3) New heat release model for Quasi-D combustion models. Similar to the motivation of developing a new ignition delay correlation, the existing heat release model is modified to account for the effect of EGR on the reaction rate of fuel, which is not being considered in the existing modeling framework proposed by Hiroyasu et al. In the modified heat release program, chemical reaction rate of the hydrocarbon oxygen mixture is included as an additional criterion to limit the rate of heat of release. This would benefit conditions at the beginning of premixed combustion with a small calculation time step, where the conventional model would result in an unrealistic spike of heat release. The inclusion of chemical reaction rate limit also improved the prediction accuracy for conditions
with EGR, where the effect of reduced oxygen concentration on the reaction rate is captured.

**Turbulent flame entrainment model for predicting NG combustion**

1) Development of the turbulent flame entrainment prediction algorithm for NG combustion in a dual-fuel engine system. This work has proposes a Quasi-D modeling framework for dual-fuel engines which incorporates both diesel spray and combustion characteristics and turbulent flame entrainment of NG. The combustion of NG is assumed to evolve from multiple ignition sites and finally engulfs the spray and propagates into the end gas zone until geometric boundaries are reached.

2) Development of flame geometry model with the fidelity to address flame interaction with boundaries. A new way of modeling the flame front area during NG flame propagation in dual-fuel combustion is proposed. The flame is assumed to initiate from the outer boundary of diesel spray and propagates into the space in the direction perpendicular to the diesel spray boundary where it starts to interact with multiple constraints including cylinder head, wall, piston and surrounding flame fronts. The proposed flame surface area algorithm solves the flame area iteratively in each main iteration of the combustion model. It also addresses the initial stage of the flame propagation, where individual flame fronts initiated from multiple ignition sites evolve, interact and form a uniform flame.
front. The algorithm incorporates geometrical information of all constraints and it can be a universal solution for various piston or cylinder head design.

3) Ignition delay correlation for dual-fuel combustion. A new ignition delay correlation for dual-fuel combustion is derived and validated. This correlation is based on the Arrhenius function based ignition correlations widely used for diesel engines. To capture the effect of reduced oxygen concentration cased by the inclusion of NG, another equivalence ratio for diesel fuel is proposed and is substituted into the ignition delay correlation. The new correlation captured this change in oxygen concentration and demonstrated better performance compared to conventional ignition delay correlations.

4) Emissions and knock predictions. The unburned NG and NOx emissions can be directly derived from the model. The NOx formation model is developed based on extended Zeldovich mechanism. The prediction of NOx is enabled by estimating the burned zone temperature, obtained from the heat release and thermodynamics sub-models. A reduced NG-air chemical mechanism is applied to predict knock in the end gas zone. The inputs to this knock prediction model are from the temperature and gas composition/property sub-models. Finally, the methane emission due to incomplete NG combustion can be obtained from the mass fraction burned profile of NG as an output of the NG turbulent flame entrainment model.

This work has provided a through description of a Quasi-D dual-fuel combustion modeling scheme that can easily be used by other researchers. The diesel fuel plays a
significant role rather than simply acting as an ignition source for the gaseous fuel. The same modeling framework can also be applied to various form of dual-fuel engines where diesel fuel only acts as an ignition source or the engine is operating at diesel only mode. By varying the number of packets and calculation time step, a balance between computing power requirement and model fidelity can be reached based on the simulation goal. The model can help expediting the calibration or development process of a dual-fuel engine, investigating new dual-fuel combustion concepts, and has the potential for real-time control applications.

System level study of dual-fuel engine with 0-D/1-D modeling approaches

1) Triple Wiebe model for analyzing dual-fuel combustion. A Triple-Wiebe combustion model is developed to represent the heat release profile of both diesel-only and dual-fuel operation. It improves the fidelity of predictions compared to a typical Double-Wiebe model, particularly the 50%-100% burned phase. Calibration of constants in the model is performed based on the experimentally determined burn rates. Values of constants are provided for a range of engine loads and speeds, which can be useful for other researchers to apply this model.

2) Improved response under transient conditions in dual-fuel operations. A source of lag in power delivery under transient load with dual fuel operation was discovered in experiments and subsequently studied using the 1-D engine system simulation. In particular, the CNG transport delay is characterized and the lag in
response can be traced back to NG transport delay. A compensation algorithm was developed for tip-in/ tip-out transients. A dynamic compensation through increased diesel injection will effectively mitigate the power lag resulted from NG transport delay during tip-in. Under some tip-out conditions, the lag cannot be fully mitigated through manipulating diesel injection profile because of signal saturation, but the algorithm performs well for most conditions.

3) A new way to derive injection parameters of a unit diesel injector. Due to difficulties in installing Hall Effect sensors to measure the needle lift in the diesel injector, a new way to derive the injection timing from cylinder pressure information and injector solenoid pulse signal was developed. A special correlation was developed to enable SOI calculation using the input from heat release profile derived from measured cylinder pressure, geometry of the injector and fuel injection signals including timing and metering pulses.

4) Analyzing dual-fuel combustion characteristics using Wiebe model. Modeling dual-fuel combustion with Triple-Wiebe functions provides an opportunity to discern the nature of dual-fuel combustion. Heat release contributions from diesel and NG are separated over a range of engine operation and NG substitution rates. Overall, dual-fuel combustion is split into four stages: premixed diesel, mixing controlled diesel, multi-site NG ignition and NG flame propagation. Predicted diesel burn rates are subtracted from the total to yield NG energy release profile. This allows estimation of heat release distribution between multi-site ignition and
flame propagation of NG. Multi-site NG ignition fraction tends to decrease with both higher NG substitution rate and NG equivalence ratio.

Physics Based Air Charge Prediction Model

In this work, a 0-D physics based crank-angle resolved intake charge prediction algorithm for real-time applications is proposed and validated. The major innovation points and contributions from this work are summarized as follows:

1) Model predicts crank-angle resolved flow through the valves and the estimate of the total mass of charge at IVC using intake pressure as a sole pressure input. The system of differential equations derived in this work enables simultaneous prediction of charge mass flow and in-cylinder pressure, thus eliminating the need for expensive cylinder pressure measurements. Thus, model is universally applicable and its application does not impose additional cost for sensors.

2) Robustness. The robustness of the air charge prediction algorithm stems from the (i) elimination of the need for in-cylinder pressure measurements which are error-prone at the low end of the range experienced during gas-exchange, and (ii) demonstrated low sensitivity to the error in intake pressure values. The latter is a consequence of the self-compensating features in the algorithm itself, i.e. ability of the algorithm to adapt the error in input thanks to the coupling of mass flow and pressure ODEs.

3) Cross-platform applications. Simulation study to investigate the application of the air charge prediction model on a VVA engine is also conducted in this work. The insights from the simulation study is that the air charge prediction algorithm
developed for a VVT engine also applies for an engine with VVA, however, additional augmentations including an additional intake temperature model and more details on the exhaust pressure are needed.

Thanks to no additional sensor cost and robustness to inputs, the air charge prediction method has great potential for real-world engine applications. It has the potential to significantly reduce calibration effort for engines equipped with multiple actuators.

**Recommendations for Future Work**

**Physics based Air Charge Prediction Model**

**Further Validation of VVA Application**

The air charge prediction model developed in this work was validated with GT-Power for VVA applications. Simulation validation shows that the modeling framework applies for VVA while some augmentations including an intake air temperature prediction model and more detailed information on the exhaust side are needed. Due to limited access to a VVA engine, this work only performed the simulation validation without doing experimental tests. Dynamometer testing and on-vehicle proving ground testing of the air charge prediction algorithm in a VVA engine is recommended for future model validation and development.

**Extension to Other Engine Platforms**
One of the objectives in developing the air charge prediction algorithm is the model should be a universal tool across engine platforms. Since the model directly estimated the flow across the valve, it inherently has the potential for cross-platform application due to its physics based nature. This work has tested its application experimentally on a conventional SI engine with VVT and EGR and also validated with a VVA engine using GT-Power simulation. Further work is recommended to extend the scope to various engine applications, including SI engines with turbocharger, EGR and VVA, diesel engines or even advanced ICEs such as HCCI engines. Once the performance is validated in all these engine platforms, this algorithm can be considered as a true universal solution.

Extend the Algorithm to Exhaust Stroke

This work has focused on the estimation of air flow across the intake and exhaust valves during the intake stroke. The modeled duration in an engine cycle starts from IVO and ends at IVC. Future work is recommended to extend the application to the exhaust stroke, where the same modeling scheme can be applied with minor modifications. This way, a physics based crank angle resolved model of the entire gas exchange process can be obtained. Significant information can be obtained from this combined model including the entire history of the gas exchange behavior between cylinder and intake/exhaust valves and a new reliable way to estimate in-cylinder trapped mass and RGF.

Intake Gas Dynamics Model
The algorithm used in the air charge prediction model requires crank-angle resolved intake runner pressure information. For conventional VVT engines, the intake runner pressure profile can be offline measured and stored as a 2-D table, where engine speed and manifold air pressure being the two table dimensions. However, when it comes to application of VVA engines or other engine types where intake gas dynamics is affected by additional engine actuators, the dimension of the intake runner pressure profile table will increase, thus multiplying the calibration effort required. Future work is recommended to develop a physics based 0-D or 1-D intake gas dynamics model with real-time potential. The objective is to output the intake runner pressure profile using available inputs while requires minimum computational power. A physics based gas dynamics model would reduce or eliminate the calibration of intake runner pressure dynamics table and it can be a universal solution across engine platforms.

Combination with Control Applications

The air charge prediction model is developed for real-time applications, thus it has a great potential to be used in control applications. One of the most promising aspect is its application in model predictive controls (MPC). The air charge model can be used as a virtual sensor and serve as input for MPC to realize optimal control. Additionally, due to its feedforward nature, steady state error may exist in its application. Especially with the aging of the engine or other changes of hardware, the accuracy of the model cannot be assured if it is feedforward only. The algorithm can be combined with adaptive controls where these steady state model errors can be eliminated through adaptation.
Dual-fuel Quasi-D Combustion Model

Further Model Validation

The Quasi-D dual-fuel combustion model developed in this work is validated with experimental data taken from the chassis dynamometer with engine in the vehicle. Due to limited experimental instrumentation, lots of information were not measured during the experiments, especially injection parameters and emissions. Additionally, the actuator sweeps at dual-fuel conditions were not complete thus only a few operating points were used for model validation. Future work is recommended to include fully instrumented dual-fuel engine tested in a dynamometer environment. Thus the model can be further validated with detailed experimental data. This would also help the development and validation of sub-models to predict the knock, emissions and unburned NG.

Development of Reactivity Controlled Compression Ignition (RCCI) Model

RCCI is a popular combustion concept among engine researchers due to its intrinsically high thermal efficiency and low emissions. The scope of this modeling work can be further extended to a development of a Quasi-D multi-zone RCCI model due to the similarities between the two combustion types. Dual-fuel combustion involves two types of fuels and two types of combustion while RCCI combustion does the same. Similar modeling framework of dual-fuel combustion can also be applied for RCCI combustion, with the emphasis shift toward the chemical mechanics.
Further Reduction of Computation Effort and Real-time Control Applications

The Quasi-D modeling approach used in this work gives its advantage in terms of computing power requirements compared to 3-D CFD modeling counterparts. However, a complete combustion simulation still requires significant computing power which is currently too demanding for real-time on vehicle applications. Due to its crank-angle resolution and in-cylinder multi zonal spatial resolution, the model needs to be iterated hundreds of times in each engine cycle. Future work is recommended to further reduce the computing effort. Possible solutions include using variable calculation step and variable number of zones to expedite the computation while maintaining the fidelity and accuracy. Once computing load is not a limiting factor, the model can be used for control applications, which would open up a new world of opportunities for further research.

In a Broader Scope

This doctoral work focuses on the physics based modeling of engines systems. The work included modeling the gas exchange and combustion processes in multiple engine platforms. The shared traits among those work is physics based modeling of engine components with reasonable computing effort. Even the gas exchange process and combustion models seem to be unrelated, they can be combined to provide a more comprehensive prediction of engine behavior and its application potential is unlimited. Specifically, the physics based air charge prediction model developed in this work has the potential to be integrated with the Quasi-D combustion model. The scope of air charge prediction model can be extended to the exhaust stroke to obtain crank-angle resolved
information of exhaust flow. This way the cylinder pressure and valve flow information during the gas exchange process can be obtained. Additionally, the output of this air charge prediction model provides initial conditions for a combustion model, while the combustion model generates the initial condition for the exhaust stroke. With combination of those two models, a real-time engine cycle cylinder pressure prediction is made possible, which has great potential for future development of engine model predictive control.
**Appendix A**

Parameters Used in the Gas Property Model

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REFERENCES


[34] EUROPE, N., 2013, "Worldwide NGV Statistics."


