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**Hydrogen/Diesel Co-Combustion in Compression Ignition Engines Through Hydrogen Ingestion and Direct Hydrogen Injection**

Helge Hening von Helldorff-Garn

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Hydrogen/Diesel Co-Combustion in Compression Ignition Engines Through Hydrogen Ingestion and Direct Hydrogen Injection

by

Helge Henning von Helldorff-Garn

A dissertation submitted to the College of Engineering and Science of Florida Institute of Technology in partial fulfillment of the requirements for the degree of

Doctor of Philosophy in Aerospace Engineering

Melbourne, Florida
May, 2021
We the undersigned committee hereby approve the attached dissertation, “Hydrogen/Diesel Co-Combustion in Compression Ignition Engines Through Hydrogen Ingestion and Direct Hydrogen Injection” by Helge Henning von Helldorff-Garn.

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Title: Hydrogen/Diesel Co-Combustion in Compression Ignition Engines Through Hydrogen Ingestion and Direct Hydrogen Injection

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This dissertation develops, implements, and validates the computational tools necessary for the computational simulation of hydrogen-enhanced Diesel combustion for premixed hydrogen charges ingested into the intake air and for direct injected hydrogen pilot charges into the cylinder. This includes a dual-fuel mechanism, a Lagrangian gaseous injection scheme, an improved spray particle breakup model, an advanced chemical kinetic reaction solver, as well as a complex n-heptane chemical kinetic reaction mechanism consisting of 35 species and 119 reversible reactions capable of describing both premixed and mixing controlled hydrogen/Diesel co-combustion at various fuel concentrations.

The results showed that low levels of either hydrogen ingestion and hydrogen direct injection can significantly improve engine efficiency by increasing the kinetic combustion reaction rates though chemical interaction of the Diesel and hydrogen radical pools and specifically though the shared interaction with H$_2$O$_2$, and by delaying the compression ignition timing, which allows for an advancement of the Diesel injection timing. This results in an increase of the premixed combustion phase, which more closely approximates the thermodynamically more efficient Otto cycle.
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To my loving wife and parents, whose unwavering and lasting support was paramount to the completion of this work.
Executive Summary

The use of hydrogen as a secondary fuel in Diesel engines has been proposed to improve engine efficiency and reduce environmental impact by previous researchers. The understanding of the mechanisms behind the ignition and concurrent combustion of Diesel fuel in hydrogen-enriched atmospheres remains limited. The objective of this work is to determine whether direct chemical interaction between the Diesel and hydrogen reactions has significant impact on the Diesel/hydrogen co-combustion, or whether physical properties such as the high flame speed of hydrogen are primarily responsible for the efficiency increases observed. The work further investigates two methods of hydrogen enrichment: pre-mixed hydrogen enrichment through ingestion of hydrogen into the intake airstream, and hydrogen direct injection.

The presented work develops, implements and verifies the necessary models for simulating dual fuel operation with a liquid and a compressible gaseous fuel in a computational fluid dynamics (CFD) solver. A gas injection model was developed based on its native liquid fuel model, in which gaseous parcels are injected in the Lagrangian domain and converted to the Eulerian gas phase. During the implementation of this model, an error in the CFD code pertaining to the coupling of the Lagrangian and Eulerian phase was discovered, the effects of which previously were erroneously attributed to the round jet anomaly of turbulence modelling. The Lagrangian gas injection model was coupled with a comprehensive 1-D compressible flow model to predict the injection velocity, discharge coefficient and mass flow rate as a function of injection pressure.
The Cascade Atomization and Drop Breakup (CAB) secondary breakup model, which represents an extension to the Taylor Analogy Breakup (TAB) model, was implemented. The CAB model differentiates between multiple breakup modes based on Weber number. The effect of the primary breakup models was investigated, and the results suggested that near the beginning of the atomization regime, both atomization and Second-Wind-Induced Breakup mechanisms are significant within the jet.

Multiple chemistry models were investigated, ranging from irreversible single-step global reactions to a significantly more complex reduced heptane mechanism consisting of 35 species and 119 reversible reactions. The direct chemical interaction between the Diesel combustion and the hydrogen combustion intermediate species was found to be of paramount significance for the accurate prediction of the mixture ignition timing. A detailed investigation of the coupled and decoupled Diesel and hydrogen reactions in a constant volume process suggest that the concurrent oxidation reactions are significantly coupled through the exchange of H$_2$O$_2$ between the two radical pools.

Utilizing these models, a parametric study was performed to compare the effects of hydrogen ingestion in the intake air with various hydrogen direct injection strategies with respect to engine efficiency. It was found that hydrogen ingestion of 6%vol can increase the indicated engine efficiency to 55%, and hydrogen direct injection under the given parameters can increase indicated efficiency to 52.3% compared to the reference case without hydrogen with an indicated efficiency of 42.66%. This efficiency increase was determined to be the result of a delayed ignition timing caused by the hydrogen, which allows for an advancement of Diesel injection timing. This effect, coupled with increased kinetic combustion rates,
consequently results in a closer approximation of the thermodynamically more efficient Otto cycle. It was found that direct injection increases the ignition delay compared to hydrogen ingestion, due to increased local hydrogen concentration, suggesting that further Diesel injection advancement and optimization is possible. The reduction of the hydrogen injection duration was shown to have a limited positive effect on engine efficiency, while early injection of the hydrogen prior to the Diesel injection event had no significant effect on the engine performance. The results suggest that a net engine efficiency gain may be achieved through both hydrogen ingestion and direct injection, even if the hydrogen is produced by power supplied by the engine itself.
Preface

In the ongoing efforts to increase the fuel efficiency of automotive engines and limit harmful emissions in order to comply with ever-increasing regulations, hydrogen has long been a primary candidate for the replacement or supplementation of conventional hydrocarbon fuels. Interest from the research community in hydrogen combustion has undergone cyclic fluctuations in focus. To this day, hydrogen combustion technologies in the automotive sector are very limited as an option to the consumer. This is partially due to alternative technologies, such as hydrogen fuel cells, and more recently the emergence of electric vehicles.

Nonetheless, the clean-burning properties of hydrogen with no carbon emissions remain a point of interest. However, considerable drawbacks exist, which have prevented hydrogen from becoming a mainstream alternative primary fuel thus far. The drawbacks include the difficulties in high-pressure cryogenic storage requirements of hydrogen, safety concerns regarding on-board storage of hydrogen in case of an accident due to the extreme volatility of hydrogen air mixtures, limited refueling infrastructure, and the fact that unlike mined hydrocarbon fuels, hydrogen must be produced from other energy sources, such as renewable electric power or more commonly by refining natural gas.

An alternative solution to using hydrogen as primary fuel, is the use of hydrogen as a supplemental or pilot fuel to conventional Diesel in a compression ignition engine. Commonly suggested, this approach involves the production of hydrogen through electrolysis by means of the power from the alternator onboard of the vehicle. The hydrogen and/or hydrogen and oxygen from the electrolysis is then introduced into the air intake
manifold. This approach alleviates the concerns regarding hydrogen refueling infrastructure, storage and onboard storage safety, as the hydrogen is produced in small quantities on demand.

This approach of introducing hydrogen into the intake air is synonymously described as hydrogen ingestion, hydrogen enrichment, hydrogen enhancement, hydrogen fumigation, or hydrogen (port) injection, and has been studied both experimentally and numerically to some extent by various researchers.

Saravanan et al. experimentally studied the effects both of hydrogen manifold ingestion and port injection at various loads. At 75% load and 12.7% hydrogen energy fraction, for hydrogen port injection a 21% increase in thermal efficiency, and an 18% efficiency increase for manifold ingestion was observed, along with a 50% reduction in CO emissions [1].

Lilik investigated the experimental performance of a Diesel engine with hydrogen ingestion under various combustion modes. Under conventional Diesel combustion, engine efficiency was slightly reduced as brake specific fuel consumption was found to increase up to 4% with increasing hydrogen concentrations of up to 15% of the total fuel energy due to displacement of oxygen in the intake charge, leading to the choking of the engine as hydrogen approached 35% [2]. The study was accompanied by computational modelling utilizing 71-species n-Heptane/NOx skeletal mechanism.

Marin found experimentally that for a small, single-cylinder, direct-injected Diesel engine at relatively low hydrogen energy fractions of 7-9%, the addition of hydrogen had
insignificant effects on brake torque and indicated mean effective pressure, and led to modest decreases in brake thermal efficiency, especially with retardation of the injection [3].

Zhou et al. stated that the effect of hydrogen addition on brake specific fuel consumption and brake thermal efficiency is highly load dependent, producing adverse effects at low to medium engine loads and positive effects at medium to high loads [4].

Demirci et al. [5] found that hydrogen addition of 0.15 to 0.6 L/min improved brake specific fuel consumption at all engine loads and by up 2.44%, while also increasing NOx production due to increased exhaust temperature. The study was performed experimentally, with the hydrogen being produced by electrolysis.

Maghbouli et al. [6] investigated the knocking behavior of hydrogen-enhanced Diesel combustion based on a computational multi-component fuel model for n-heptane and toluene, which predicted knocking to occur at and above hydrogen charges of 5% by volume.

Mobasheri et al. utilized the ECFM-3Z combustion model, which differentiates between combustion zones based on local equivalence ratio to apply different quasi-global combustion reactions [7]. In their computational research, they investigated the effects of the addition of hydrogen and nitrogen to the intake charge, showing significant reductions in CO (-54%), CO2, and soot (-89%) but increases of NOx (+75%) emissions when 8% by volume hydrogen was introduced while reducing the amount of Diesel fuel accordingly [8].

Liew et al. experimentally investigated hydrogen-Diesel combustion on a Cummins ISM 370 engine, finding that at 70% load relatively large amounts of hydrogen, on the order of 30% of the total fuel energy, were required to produce significant effects on the cylinder pressure.
and combustion process [9], [10], but noted significant increases in the power output. The experimental results of these studies are used as reference data for some of the computational work presented in this dissertation. Computational studies based on these works were further published by Shojae et al. [11] and Yang et al. [12], both of which utilized single-step global combustion models.

The large variability and, in some cases, contradictory findings among these literature findings due to the load dependence of the effects of hydrogen, as well as the wide range of operational parameters and specific engine performances, the range of hydrogen energy fraction etc., considered by the various studies makes these results difficult to compare. However, in their review of this technology, Alrazen et al. [13] note that the majority of researchers report a positive effect of hydrogen addition on thermal efficiency and fuel consumption. Further, aside from general statements that hydrogen enrichment improves the flame speed, combustion process, and ignition characteristics, a review of the available literature does not provide much detailed insight into the mechanism by which hydrogen addition interacts with the Diesel combustion to produce the described effects.

A significant drawback preventing the use of hydrogen enrichment of the intake air is that despite relatively low hydrogen fractions, large amounts of hydrogen are needed to provide a homogeneous air/H2 mixture, which may exceed the amount of hydrogen that can practically be produced on demand on-board. While the need for large hydrogen amounts can be reduced by selectively only utilizing hydrogen during, for example, high power demand driving conditions, an alternative approach might be the stratification of the hydrogen charge similar to liquid fuel direct injection. This would allow for higher hydrogen
concentrations and their strategic placement within the cylinder to increase the beneficial effects of the hydrogen while reducing overall hydrogen demand by the engine.

The objective of this dissertation is therefore to develop and implement the necessary computational models for dual fuel capabilities and compressible hydrogen injection models, the chemical models to assess and compare pure Diesel combustion with hydrogen enhanced Diesel combustion through intake ingestion of hydrogen, as well as direct hydrogen injection into the cylinder. The combined models are then demonstrated in a parametric study to quantify the effect of the hydrogen ingestion versus several hydrogen direct injection strategies on engine efficiency. A full optimization of the hydrogen direct injection, as well as the physical design of the injector fall outside the scope of this work.

About KIVA

The KIVA code set has been a defining program in the establishment of the modelling of fuel sprays and simulation of internal combustion engines [14]. KIVA is a computational fluid dynamics (CFD) code that was originally developed by the Los Alamos National Laboratory, specialized for modelling transient, three-dimensional, chemically reactive thermal flows of internal combustion engines. The mass, momentum, and energy equations are discretized in time and space, where KIVA utilizes the Arbitrary Lagrangian-Eulerian (ALE) finite volume method [14] [15] for the spatial differencing. The solution for the moving mesh is achieved by dividing the process into three “Phases”. Phase A denotes a Lagrangian description of the particle phase, which includes spray droplet motion, collision and breakup. In Phase B, the Lagrangian motion of the flow field is calculated, such that the vertices move with the flow field velocity and no convection through cell faces occurs. In
the Eulerian Phase C, the flow field is remapped to an updated computational mesh by convecting the material across the computational mesh boundaries.

The code set utilized for the work presented here is a modified version of KIVA-3V release 2. The major modifications to the code are briefly outlined below.

a) Dual fuel capabilities for gaseous fuels were added by introducing a modified copy of the liquid fuel definition, injection, evaporation and coupling subroutines. The modifications necessary for proper performance of the injection and coupling subroutines are outlined in additional detail in Chapter 1. The injected secondary fuel is added under a dummy species label, which allows separate tracking of injected versus otherwise present amounts of the same species. The injected species parcel is immediately converted to the Eulerian regime by utilizing the evaporation mechanism. Optionally, the dummy species is then added to the actual target species and the dummy species is reset.

b) An improved particle break-up model was implemented, details of which are outlined in Chapter 3.

c) CHEMKIN is a kinetic chemistry solver software originally developed by Sandia National Laboratories, that sets up and solves the fully coupled ordinary differential equations for complex kinetic reaction mechanisms [16]. The CHEMKIN chemistry solver was fully implemented as a replacement option to the native KIVA chemistry solver. Utilization of this solver requires the user to supply the chemistry mechanism binary file, which is obtained by the CHEMKIN preprocessor and in turn requires the CHEMKIN mechanism file and thermodynamic data file. The input from the
CHEMKIN binary file overwrites the KIVA input data for species definitions. CHEMKIN is called for each cell at each time step. The current chemical gas composition of the cell is parsed to CHEMKIN, which sets up the coupled differential equations, solves these for a constant volume reaction, and the returns the updated chemical composition to KIVA.

d) The native KIVA solver was extended in functionality to address third-body reaction and pressure dependent reactions for both Lindemann form cases and non-Lindemann form cases, both of which translate unimolecular reactions into rate constants for two representative elementary step reactions suitable for chemistry solvers.

e) Numerous changes for stability of the code were made, such as improving expressions that can potentially lead to array overflows. For example, in the original code, liquid fuel properties such as surface tension, are only defined up to their respective critical temperatures. In rare cases, a very small liquid particle may impact a wall and have the resulting heat transfer result in the fuel property tables being exceeded. Specific checks for such cases were implemented, as the resulting array overflows can lead to significant errors or crashing of the simulation.
Chapter 1
Computer Modelling of Gaseous Injection

In this chapter, the methodology for introducing a compressible gaseous fuel into a computational domain through a Lagrangian parcel injection model with subsequent conversion to the Eulerian gas phase is developed, implemented and verified through comparison with experimental literature data.

The contents of this chapter have previously been substantially published by this researcher under the title “Gaseous and Liquid Jet Direct Injection Simulations Using KIVA-3V” in the Journal of Multidisciplinary Engineering Science and Technology (JMEST), Vol. 6 Issue 1, January 2019, ISSN: 2458-9403. [17]

1.1. Introduction

Liquid injection algorithms have been thoroughly studied and verified for both internal combustion and gas turbine engine simulations, and have been an integral part of many computational fluid dynamics (CFD) codes for decades, yet similar gaseous injection models capable of describing injector type compressible gaseous jets are often lacking.

CFD codes can be roughly grouped into two classes: scientific research type codes and engineering application type codes. Scientific-level codes generally utilize advanced methods such as Direct Numerical Simulation (DNS) to resolve all phases at all length scales and are inherently much more accurate than engineering level codes [18]. DNS requires an extremely fine mesh, resulting in high computational memory and processing power.
requirements and impractically long computational times. Engineering level codes, on the other hand, often rely on sub-models to describe phenomena not resolvable on a relatively coarse length scale, as well as commonly utilizing Lagrangian phase calculations to describe the particle phase [19].

The motivation for this work was the need for a gaseous jet injection model for engineering level CFD calculations, that could adequately describe the macroscopic characteristics of a gaseous jet plume, where the injector nozzle is much smaller (about two orders of magnitude) than the computational domain. For scientific level codes, this disparity in scale is generally resolved by explicitly modelling the internal flows of the injector without much additional penalty, as fine mesh sizes are already required by such techniques. Engineering level codes may also explicitly model the internal flows and utilize advanced dynamic meshing techniques to reduce the cell count in the main computational domain (e.g. engine cylinder). However, the injector size is often on the order of less than 1 mm diameter and thus would require a mesh size on the order of 0.01 mm to accurately resolve the flow, while the cells in the engine cylinder is commonly on the order of 2 mm. The injector modelling thus presents a significant penalty on the computational speed due to the large number of cells required to explicitly model the internal flows inside the injector. Also, the interface between drastically different mesh sizes presents challenges and often leads to the introduction of additional error especially at the interface between differently sized cells [20].

Alternatively, gaseous injection has historically often been achieved by manually specifying individual cell faces as inlet boundaries. This approach was used by Ouellette [21], [22] to study the direct injection of natural gas in Diesel engines. In addition to being cumbersome,
this method requires perfect match between the inlet boundary mesh size and injector inlet area to be modelled to ensure correct mass flow rates, and thus does not allow for changes in the mesh setup, as would be required for mesh sensitivity studies.

The methodology of utilizing the liquid injection subroutine for gaseous injections was first published by Hessel et. al. under the term “Gaseous Sphere Injection” [23] and compared to the experimental data by Witze [24], [25]. The gas was injected as parcels in the Lagrangian particle domain and prevented from converting to the mixed Lagrangian-Eulerian fluid or “gas phase” while near the injector. After a prescribed distance from the injector, the parcels were converted to the gas phase utilizing the KIVA evaporation algorithm such that the entire parcel was instantly added to the gas phase. Since the Lagrangian particles are chemically non-reactive in KIVA, this has significant impacts especially on the near injector fuel ignition in engine simulations. Further, turbulent kinetic energy was artificially reduced within the jet plume according to the empirical relationships presented by Witze. These two modifications introduced several input variables, which required model tuning to achieve agreement with the experimental data. This same model was used by Choi et. al. for a compressed natural gas (CNG) direct injection study [26].

The gaseous injection model presented in this paper utilizes the same gaseous spherical injection methodology without the need for the artificial phase conversion delay and the modifications to turbulent kinetic energy, which were needed by Hessel to achieve agreement between the experimental and computational results. While the approach of the work presented here remains the same, a correction and improvement to the previous injection model is presented, as well as describing the capabilities and limitations of the
Lagrangian parcel injection model in a novel context, i.e., its applicability to direct gas injections. The model is simple to implement, negates the need for explicit modelling of the internal injector geometry, is relatively robust against mesh changes, and correlates well with experimental results, while not requiring the introduction of any model tuning constants to achieve agreement with the experimental results.

1.2. Simulation

All simulations presented in this chapter were performed using KIVA 3V release 2 on a Linux personal computer. The mesh consisted of a 3x3x6 cm volume, as described by Table 1-1 and depicted in Figure 1-1, consisting of ambient air at 1 atm pressure and 300 K. The domain dimensions were chosen to avoid any wall boundary effects, as was verified by the results. Further, the bottom boundary was modelled as an outflow boundary to maintain constant pressure within the test volume.

![Figure 1-1: Computational mesh setup](image-url)
The gas was injected directly downwards from the top center of the volume. In this case, air was injected into ambient air. However, within the simulation the injected air was treated as a separate species to differentiate it from the ambient air for post processing. Each simulation was carried out for 8 ms with gas being injected using a square wave injection profile for a duration of 4 ms beginning at the start of the simulation. The injection velocity of 103.5 m/s and injection mass of 0.5529 mg were defined as input parameters to represent the experimental and computational setups by Witze and Hessel respectively, negating the need to specify injection pressure, which was not specified in the experimental literature. The injector was a single-hole, straight bore injector of 0.6 mm radius. The wall temperatures and injection temperature were both set to a constant value of 300 K.

The gaseous injection was achieved by utilizing a modified set of the KIVA fuel injection subroutines. The injection gas is quantified in the fuel library based on the thermodynamic properties calculated by assuming atmospheric air with volume fractions of 79% nitrogen and 21% oxygen and utilizing the thermodynamic data presented by Vargaftik [27]. For gaseous species, a “liquid density” is defined within the fuel library, which is largely immaterial for the injection process since the injection mass and velocity are specified and thus only influences the number of parcels injected at each time step. The low critical temperature of the gaseous species triggers an immediate and complete conversion of the gaseous parcels from the Lagrangian particle phase to the gas phase through the KIVA evaporation and phase coupling subroutines as soon as the parcel enters the computational domain. The simplicity of implementation of this approach compared to manually identifying injection cells and setting them to inflow boundaries is a major benefit of the
method, especially when multiple injectors are modelled. Table 1-1 outlines the details of the various cases presented here.

Table 1-1: Description of Case Details

<table>
<thead>
<tr>
<th>Case</th>
<th>Mesh size $dx=dy=dz$ [mm]</th>
<th>Nr. of mesh cells $nx/ny/nz$</th>
<th>Computational Time [min]</th>
<th>Turbulence Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.500</td>
<td>20/20/40</td>
<td>5.32</td>
<td>RNG</td>
</tr>
<tr>
<td>2</td>
<td>1.000</td>
<td>30/30/60</td>
<td>29.77</td>
<td>RNG</td>
</tr>
<tr>
<td>3</td>
<td>0.750</td>
<td>40/40/80</td>
<td>131.12</td>
<td>RNG</td>
</tr>
<tr>
<td>4</td>
<td>0.625</td>
<td>48/48/96</td>
<td>321.61</td>
<td>RNG</td>
</tr>
<tr>
<td>5</td>
<td>0.625</td>
<td>48/48/96</td>
<td>321.30</td>
<td>Std. K-Epsilon</td>
</tr>
</tbody>
</table>

1.3. Erroneous Results Using Unmodified Kiva

The attempt to recreate the experimental results by Witze and the corresponding computational results by Hessel using an unmodified version of KIVA 3V release 2, revealed several inconsistencies in the result. While the results for axial velocity utilizing the mesh size described by Hessel appeared promising at first, a high inverse mesh dependency was observed. In general, one would expect the quality of computational results to improve with increasing mesh density. However, in this case it was found that computational results appeared to converge only with increasingly coarse meshes and diverged from the experimental results as the mesh was refined. This is shown in Figure 1-2, which depicts the interpolated centerline velocity at the first probe point 2.9 mm from the injector for various mesh sizes, where the centerline velocity should be roughly 85 to 90 m/s as seen from the experimental data depicted in Figure 1-7.
Specifically, the refinement of the mesh caused the axial centerline velocity to be severely overpredicted in individual cells as cell size was reduced below 2 mm, to the point where velocities near the injector significantly exceeded the prescribed injection velocity of 103.5 m/s. This trend appeared to continue in an exponential fashion as cell size was further reduced, producing clearly non-physical, erroneous results. It should be noted that the values depicted in Figure 1-2 are interpolated values for the probe point and individual vertex values were even higher for all cases. The apparent convergence at coarser mesh sizes is due to the reduced impact of the injected gas on the larger cell mass of the coarser mesh.

It should further be noted that the use of centerline velocity in this context has severe limitations for comparison. Due to the nature of finite volume computations and similarly experimental measurements using hotwire anemometers, the exact peak centerline velocity
cannot be measured due to the finite length scales of the mesh size and hotwire anemometer. Instead, in both cases an average value capturing the centerpiece of the Gaussian radial velocity distribution, as depicted in Figure 1-3, is obtained. This will cause an under-prediction of the centerline velocity, especially when the mesh size is large compared to the jet radius, and in particular close to the nozzle where the radial velocity gradient is largest. It is thus expected that the calculated and measured centerline increases as mesh size is refined and the size of the hotwire anemometer reduced. However, in no case can this effect account for a predicted velocity larger than the jet injection velocity, as was produced by the unmodified KIVA code. These results are thus clearly erroneous and requiring the underlying source of this error to be investigated.

Figure 1-3: Characteristic structure of an ideal axisymmetric turbulent jet [25]
The results further showed asymmetrical jet behavior. Further investigation and overlaying of the mass fraction and velocity profiles clearly depicted an offset between the mass and momentum contour outlines, which was identified as the cause for the asymmetrical jet behavior. Figure 1-4 demonstrates this for the coarse mesh used in Case 1 with arbitrary contour levels to aid in the visualization. The left (red) mass fraction plume and the right (blue) velocity profile plume are clearly offset and originating from different locations, as well as differing in shape. Specifically, analysis of the raw data showed the mass plume to originate from the cell center and the velocity plume originated from one of the corresponding vertexes.

Figure 1-4: Mass (red) and Momentum (blue) Plume Offset (zoomed in mesh cross-section), jet originates at top center
1.4. Corrections to KIVA

To understand and correct the root cause of the issue described above, the KIVA algorithm needs to be understood. KIVA utilizes Lagrangian particle tracking in the Cartesian coordinate system (denoted as the “particle phase”). Information such as location, mass, velocity, temperature etc. are stored in reference to each particle, and are not bound to any mesh cells or vertex.

The fluid or “gas phase” is defined by a mixed Lagrangian-Eulerian description, where the governing equations are solved through a modified Arbitrary Lagrangian-Eulerian method (ALE). Being a finite volume method, the ALE method utilizes primarily cell center based quantities, such that mass, momentum, internal energy etc. are stored at each cell center. However, KIVA utilizes cell-faced velocities, which is done to minimize parasitic velocity modes. Thus, unlike the cell center based quantities, the velocities are stored at each cell vertex.

The gas phase is thus described by a single explicit mesh defined by its vertices, where each cell vertex is labeled \(i\) through \(i_8\). The front left bottom vertex \((i_4)\) of each cell is used as the reference vertex to identify the current cell. Additionally, an offset implicit mesh of “momentum cells” is defined based on the regular vertices, in which 1/8th of each momentum cell overlaps each of the neighboring regular cells. The momentum cells are utilized in the differencing of the momentum equation, and are referenced by identifier “imom”, which lies at the center of the momentum cell and at the vertex of the regular cell. A visualization is provided in Figure 1-5. For more detailed information, the reader is referred to the KIVA 2 manual [14].
The issue arises in properly distributing the mass, momentum, and energy of the Lagrangian parcels to the gas phase mesh. In the unmodified KIVA process, the regular cell containing an evaporating parcel is identified and the parcel mass and internal and turbulent energy are added to the center of the cell.

Similarly, the momentum cells in which the parcel is located is identified, and the momentum of the evaporated parcel is added to this momentum cell. However, the momentum cell and regular cell are offset from each other. Thus, the momentum is added to a slightly different location in the mesh than the corresponding mass. When the mesh size becomes sufficiently coarse or the mass and momentum become sufficiently large compared to the undisturbed gas phase cell, this creates notable inconsistencies in the location of the mass and momentum jet plumes, as well as creating false asymmetric behavior in the solution.

Figure 1-5: KIVA naming conventions for cell identifiers
The issue is further exacerbated by the fact that the velocity at each vertex is a derived quantity. KIVA tracks momentum by solving the momentum equation. Velocity at each vertex is calculated by dividing momentum by mass. In the unmodified KIVA code, this is achieved by defining an auxiliary vertex mass, \( m_{\text{vertex}} \), which is simply 1/8th of the corresponding cell mass.

However, since the momentum was deposited at the momentum cell, the location of which corresponds to a singular of the eight vertices, a mismatch between the momentum and mass considered for this calculation is experienced. In effect, a singular vertex receives the entire parcel momentum, which is then divided by 1/8th of the parcel mass, such that velocity, \( u \), at that vertex \( i4 \) at time \( t \) is given by the momentum at the vertex, \( P \), and the vertex mass, \( m_{\text{vertex}} \).

\[
\begin{align*}
  u^t_{i4} = & \frac{P_{i4}^{t-1} + P_{\text{parcel}}}{m_{\text{vertex \ i4}} + \frac{1}{8}m_{\text{parcel}}} \\
\end{align*}
\]  

(1.1)

Thus, the velocity is highly overpredicted at this vertex. The other vertices of the regular cell receive no additional momentum contribution from the evaporated parcel, yet the previously existing momentum of these vertices is still divided by an auxiliary vertex mass that was increased by 1/8th of parcel mass. This results in a diminishment of the momentum and thus velocity at these vertices. In this case, the velocity is incorrectly described as

\[
\begin{align*}
  u^t_{i4} = & \frac{P_{i4}^{t-1}}{m_{\text{vertex \ i4}} + \frac{1}{8}m_{\text{parcel}}} \\
\end{align*}
\]  

(1.2)
To summarize, a discrepancy between the location of mass and momentum contribution from evaporating parcel was found, as well as a discrepancy between the momentum and respective auxiliary vertex mass used to derive the vertex velocities. It is suggested that the KIVA code should be modified to ensure that any momentum contribution from evaporating parcels is attributed to the same location in the mesh as its corresponding mass addition to the gas phase, such that the velocity at each vertex of the cell containing the evaporating parcel is described as

$$u_{i4}^t = \frac{p_{i4}^{-1} + \frac{1}{8} P_{\text{parcel}}}{m_{\text{vertex} i4} + \frac{1}{8} m_{\text{parcel}}}$$

(1.3)

Fortunately, the issue is easily rectified through the following corrections:

1) In subroutine \textit{pcouple} the following lines (generally located in loop 30) must be extended for all vertices, \texttt{i1} through \texttt{i8}, and modified such that each vertex receives 1/8th of the parcel momentum contribution (\texttt{ru/rv/rw}) in accordance with the mass distribution. This requires redefining these vertices (\texttt{i1} through \texttt{i8}) relative to \texttt{i4} within the loop.

$$u(i4)=(u(i4)-ru (i4)) \times \text{srcmv}$$

$$v(i4)=(v(i4)-rv (i4)) \times \text{srcmv}$$

$$w(i4)=(w(i4)-rw (i4)) \times \text{srcmv}$$
2) The conversion from momentum to velocity (*srcmv in the lines above) must be separated from the loop and performed separately by introducing an additional loop to avoid multiple applications of the conversion factor, since every vertex is now addressed up to eight times.

3) In subroutine *pmom* (generally loop 30), the identifier *imom* must be changed to *i4* in the lines calculating *ru* (shown below), *rv*, *rw* and *suvw*.

\[ ru(imom)=ru(imom) + partrm* (rdenr3*(upt+dragdt*uprime)- radp3*upt) \]

This will ensure that the same cell is chosen for both the mass and the momentum contribution.

It should be noted that these lines of code reflect the unmodified KIVA code to aid in the identification of the lines of code that require changes and do not reflect application of the necessary changes mentioned above.

It should further be noted here again that in this study the injection subroutines in KIVA were utilized for purposes other than their intended purpose of only liquid injection. In gaseous injection, all parcels are immediately converted to the gas phase through the evaporation subroutine. Since all mass and all momentum are added to a single cell, and parcel mass may no longer be much smaller than the undisturbed cell mass, the described effects are much more pronounced than ordinarily experienced in liquid injection and evaporation processes. During liquid injection, mass and momentum contributions are generally small compared to cell mass and dense uniform sprays will likely result in each vertex receiving momentum contributions from parcels in the neighboring cells, further
masking the issue. The effect of the described issue is thus much less pronounced in evaporating liquid sprays, while addressing the issue for gaseous injection simulations is much more crucial. Nonetheless, it is recommended to apply these changes for liquid injection simulations as well.

Previous researchers, such as Nordin [28], have investigated more sophisticated momentum coupling approaches, such as weighting the momentum to the inverse of the distance between the parcel location and the vertices. Such inverse distance weighting was investigated as part of this research but deemed fundamentally unworkable in the context of the KIVA code, as any weighting of the momentum would also imply a non-uniform mass distribution within the cell, which is impossible without additional subgrid models.

Abani and Reitz [29], [30] also investigated the momentum coupling of spray parcels with the gas phase, but focused mainly on particle-particle interactions by developing a model based on an effective injection velocity derived from Helmholtz’s vortex motion analysis. They did, however, not address the momentum deposit location issue in the coupling model that is described in this work.
1.5. Results

The velocity profiles presented in Figure 1-6, Figure 1-10, Figure 1-11 and Figure 1-15 were obtained by interpolating the adjacent vertex values to obtain the quantities at the probe points. Each line represents the axial velocities at a specific distance of the probe point from the injector along the centerline of the jet.

The steady-state plateau velocities at the jet centerline in Figure 1-6 show overall good agreement with the experimental results by Witze depicted in Figure 1-7 and the computational results by Hessel et. al depicted in Figure 1-8.

The computational results show a slight over-prediction of axial velocity near the injector nozzle compared to the experimental results. This may be explained by the limitations of the experimental setup due to the finite size of the hotwire anemometer of 1 mm. In the near nozzle area, the probe size exceeds the jet core size, thus capturing the effects of diminishing velocities at the edge of the parabolic jet velocity profile and leading to overall reduced velocity readings. Further from the injector, the computational axial velocities results are within the experimental scatter.

The computational results show a markedly faster response to the initiation and termination of the jet in the near-injector region than in the experimental results in Figure 1-7. The difference is easily explained by the response time of the opening and closing of the injector valve, which is not modelled here and instead represented by the immediate response of the modelled square wave injection profile.
Figure 1-6: Computational centerline Velocity Case 4, fine mesh with RNG model
Figure 1-7: Ensemble-averaged measurements of the starting-jet centerline mean velocities by Witze [24], [25]

Figure 1-8: Computational centerline velocity results by Hessel et. al. [23]
The jet penetration, as observed by the flow acceleration at each probe point and represented by the timing of increasing slopes of the velocity profile, further show good agreement with the experimental results, as well as a marked improvement over the significantly delayed values observed in the computations by Hessel. Further, the non-dimensionalized jet penetration in Figure 1-9, as defined by the time to reach 70% of the steady state velocity, shows near perfect agreement for Case 4, compared to the experimental data best fit line. Here \( u_j \) denotes the jet exit velocity in m/s, \( r_j \) denotes the effective nozzle radius of 0.69 mm and \( t_j \) denotes the jet time constant of 7.0 \( \mu \)s.

All computational results in this plot are slightly translated in the time axis compared to the experimental best fit line because the experimental time zero is set at the time the injector is fully opened, not accounting for the finite opening time of the injector. This is evident from the original experimental data, which shows a positive jet penetration at time 0.

The coarser meshes of cases 1, 2 and 3 result in a reduction of jet penetration with cases 2 and 3 still being fairly accurate. The difference is mainly attributed to the reduced centerline velocity near the injector nozzle resulting from the smearing of the jet with the surrounding quiescent volume. Additionally, the coarser mesh may contribute to this effect, as the jet plume has to traverse an increased distance between vertices and it may take several time steps before the jet is reported at the next cell.
Figure 1-9: Tip penetration distance as a function of the square root of time elapsed from initiation of the jet with experimental results by Witze [24], [25]

Figure 1-10 depicts the same case as discussed above, except with a significantly coarser mesh. While the plot is qualitatively similar to the fine mesh case, quantitatively the centerline velocities are significantly under-predicted near the injector. However, the far field centerline velocities are remarkably well captured. The same trend is observed for cases 1 and 3. Even the extremely coarse mesh of case 1 in Figure 1-11 manages to fairly accurately depict the far field velocities, especially when keeping in mind the drastically reduced computational time for this case, despite the large deterioration of the near-injector velocities. This is explained by the fact that the total jet momentum is identical for all cases despite differences in average cell velocities.
Figure 1-10: Axial Velocity Case 2, coarse mesh with RNG model

Figure 1-11: Axial Velocity Case 1, extremely coarse mesh with RNG model
Figure 1-12 and Figure 1-13 depict the velocity and mass fraction profile cross section at the jet centerline respectively. Each of these plots represents 3.5 ms after the start of injection, which marks a point where all probe points are at their respective steady-state velocity. In both the mass fraction and velocity plots, a severe blurring of the gradients can be observed with the very coarse mesh in case 1, as well as a slightly reduced jet penetration and correspondingly increased jet spreading. As expected, the correct prediction of these gradients is improved with the refinement of the mesh, to the point that case 3 and 4 are practically indistinguishable. However, the macroscopic qualities of penetration and spreading of the jet plume show little variation between all cases. This smearing of the solution is unavoidable with coarse meshes and would also be present if the gas was introduced through a boundary surface.

Figure 1-12: Velocity Profiles
Finally, Figure 1-14 depicts a visualization of the velocity profile of a fully developed jet produced in MatLab based on the empirical model proposed by Witze [25], which shows good agreement of the momentum spreading rate of the jet compared to case 4 in Figure 1-12. It should be noted that the empirical model proposed by Witze assumes constant jet velocity within a distance of 12.5 times the injector radius, or 7.5 mm in this case. This explains the more pronounced high velocity core near the injector. Unlike the starting jets depicted in Figure 1-12, the empirical model depicts a fully developed steady state jet, explaining the higher velocities in the far field and reaching the lower edge of the domain. Thus, conclusions can only be made on the spreading angle, while the penetration distance is not comparable with the other results. However, both the empirical velocity profile in Figure 1-14 and the predicted velocity profile for case 4 in Figure 1-12 display an initial spreading angle of about 16 degrees and thus show excellent agreement.
Figure 1-14: Fully developed velocity profile according to empirical model by Witze [25]

1.6. Effect of Turbulence Model

The turbulent round-jet/plane-jet anomaly is a well-known and well-documented issue describing a roughly 40% over-prediction in spreading rate, along with the associated reduction in penetration length, when modelling round jets using the standard k-epsilon turbulence model [31]. Many improved turbulence models, such as the RNG-k-epsilon model [32], [33], which was implemented in the KIVA-3V code on release 2 [15], and the
Realizable k-epsilon model [34], which addresses the round jet anomaly particularly well, have been developed.

While the standard k-epsilon model only accounts for turbulence production of a single length scale, the RNG k-epsilon model utilizes renormalized group theory to take into account different length scales and only systematically removes the smallest length scales to achieve resolvability of the model, leading to improved model performance. A further benefit is that the model constants can be explicitly calculated using the RNG approach [35], thus negating the need for model tuning.

Figure 1-15: Axial Velocity Case 5, Fine mesh with standard K-Epsilon model
Given the common round-jet anomaly problem, the discrepancies encountered due to the issues in the KIVA momentum coupling described above can easily be misinterpreted as turbulence modelling issues. Figure 1-15 compares the axial velocity profiles using the same refined mesh as case 4 for the standard k-epsilon model and the RNG k-epsilon model.

It is apparent that the axial steady state velocity is significantly reduced at all probe locations. Similarly, Figure 1-9 shows a significant reduction in jet tip penetration for case 5. Further explanation can be gleaned from the velocity cross section profile for case 5 in Figure 1-12 and the mass fraction profile in Figure 1-13, which clearly show a significantly increased spreading rate of the jet near the injector with an initial spreading angle of about 22 degrees, as compared to the 16 degree initial spreading angle of RNG simulation and the empirical results. The high velocities near the injector along with the overestimate of the turbulence values of the k-epsilon increase turbulent mixing and spreading rate while quickly diminishing the high velocity cone at the jet centerline, which is still present in the RNG k-epsilon cases.

Given the presented results for cases 1-4 with respect to jet penetration and spreading angle, it was determined that the RNG k-epsilon model adequately describes the turbulence of the round jet in this case and that no further introduction of more sophisticated turbulence models or other means of artificial turbulence reduction, such as presented by Hessel, were necessary.
1.7. Conclusions

It was demonstrated that the liquid injection subroutines may be utilized for gaseous injection modelling with only minor modifications, which leads to a fast implementation time.

It was shown that this methodology allows for the accurate simulation of round gaseous jets, as long as the mesh size near the injector and jet core is on the order of the injector radius, in order to capture the smallest feature of interest which in this case is the jet core velocity and mass distribution.

The macroscopic characteristics of the jet plume, including jet penetration and spreading angle, were reasonably well preserved far from the injector even as a coarser mesh size was used. A coarser mesh may be utilized if the near injector characteristics are not of great importance and no chemical reactions are modelled, such that mass fractions are of lower significance. Thus, in many cases a significant reduction in computational times may be achieved while maintaining adequate solution quality of the macroscopic jet plume characteristics.

As the mesh size becomes coarser, the high velocity and mass fraction gradient are lost due to smearing of the solution gradients. Especially for chemically reacting flows, the mass fraction gradient will have significant effects on the chemical reaction rates and thus a refined mesh near the injector on the order of the injector radius is necessary.

The injection methodology described in this paper does have some drawbacks. The algorithm will always center the injector location on the injection cell. This may lead to difficulties accurately positioning the injector within the mesh, especially with very coarse
meshes. This may be remedied by refining the mesh at the injector location. Additionally, if multiple injectors/injector holes are modelled, each injector requires all 8 vertices of the injection cell without overlap to other injection cells in order to avoid cancellation of the momentum of opposing jets.

Modifications to distribute the parcel momentum to each vertex on the basis of the inverse distance-from-the-injector weighting instead of even distribution to all 8 vertices was deemed fundamentally unworkable in the context of the current KIVA code, as this introduces the invalid assumption of non-uniform subgrid mass distributions, which would require extensive modifications to KIVA.

It was found that upon the correction of the momentum coupling process, the RNG k-epsilon model described the jet characteristics well and adequately addressed the round jet anomaly compared to the standard k-epsilon model. Thus, no additional modifications to the turbulence model were deemed necessary. This negates the necessity to introduce additional tuning constants to the model. Further, by immediate conversion of the parcels from the particle phase to the gas phase, and due to the relatively large size of the parcel volume compared to the cell volume, the mass fractions in the near injector area are well captured.

A significant flaw regarding the momentum coupling of the particle phase with the gas phase affecting both gaseous injection and evaporating liquid injection processes was discovered within KIVA. The simple modifications necessary to address this issue were outlined in detail. It is highly recommended that researchers utilizing KIVA or any KIVA derived codes verify that this issue does not pertain to their softwares and/or resolve it accordingly.
Chapter 2
1-D Compressible Injection Model

This chapter discusses the development, integration and verification based on available literature data of a comprehensive 1-D compressible gas injection model for use with the previously introduced Lagrangian parcel injection methodology. The model takes into account the real world effects of compressibility on density, viscosity, compressibility factor, and discharge coefficient in order to estimate injection velocity and mass flow rates for a given injection pressure ratio.

The contents of this chapter have previously been substantially published by this researcher under the title “A Comprehensive Compressible Injection Model for High Pressure Gaseous Fuel Injectors” in the Journal of Multidisciplinary Engineering Science and Technology (JMEST), Vol. 6 Issue 2, February – 2019, ISSN: 2458-9403. [36]

2.1. Introduction

The Lagrangian parcel gas injection methodology based on the KIVA liquid injection routines introduced in the previous chapter utilized mass flow rate and injection velocity as input variables, which is numerically the simplest methodology of describing the injection process. At this point, a significant disconnect between the experimental and computational approach exists, as experimentally these quantities are difficult to assess and experimentally measure and generally not reported in many experimental studies, which instead rely on the experimentally easily obtainable pressure differential across the nozzle to describe the injection conditions.
Previously, Micklow et. al. [37] extended the capabilities of the KIVA-3V code set by basing the injection parameters, i.e. injection velocity, mass flow rate, particle size etc. solely on the injection pressure ratio and reservoir gas state. The injection velocity is updated at every time step, and the corresponding mass flow for the time step is found simply through the application of the incompressible form of Bernoulli’s equation and the continuity equation.

\[ v_{inj} = \sqrt{2\frac{(P_0 - P_{cyl})}{\rho_{liq}}} \]  

(2.1)

\[ m = C_d A \rho_{liq} v_{inj} \]  

(2.2)

Since the previous model my Micklow et. al. is only valid for liquid, incompressible fuel sprays, a further extension is required for compressible gaseous injections. This compressible model must include compressibility effects along the nozzle geometry, compressibility effects on the gas characteristics such as density and viscosity, as well as compressibility effects on the geometry-based discharge coefficient. To account for these effects, a comprehensive compressible 1-D model was developed to predict the injection velocity and mass flowrate under the conditions of a time-varying pressure ratio to negate the need for extensive experimental data at various pressure ratios. This comprehensive model represents a combination of previously established sub-models addressing each of the aspects described above.
2.2. Computational Model

2.2.1. Compressible Discharge Coefficient

Borrowing from the work of Jobson [38], who presented an analytical investigation of the effects of compressibility on flow through orifices and nozzles, the following model was amended and discretized for utilization within the KIVA environment. The following expressions for injection velocity and mass flow rate (eqn. 2.3 - 2.5) under subcritical conditions are convenient, as they only require prior knowledge of the injection reservoir quantities, with the exception of the pressure ratio across the nozzle, \( r \), which requires the experimentally easily obtainable in-cylinder pressure. A description of the variables used here can be found in the nomenclature section at the end of this chapter.

\[
\begin{align*}
  v_{inj} &= \frac{K_N}{r^{\frac{\gamma}{\gamma - 1}}} \sqrt{\frac{P_0}{\rho_0}} \quad \text{(2.3)} \\
  \dot{m} &= C_d K_N A \sqrt{\frac{P_0}{\rho_0}} \quad \text{(2.4)} \\
  K_N &\equiv \frac{2 \gamma r^{\frac{\gamma}{\gamma - 1}}}{\sqrt{\gamma - 1}} \left( 1 - r \left( \frac{\gamma - 1}{\gamma} \right) \right) \quad \text{(2.5)}
\end{align*}
\]

For choked flow, the analytical model further simplifies to (eqns. 2.7 – 2.9), as the critical pressure ratio remains constant. However, as the subcritical expressions for \( K_N \), \( u \) and \( \dot{m} \) remain valid, explicit implementation of these formulas is not necessary, as long as the pressure ratio variable is limited to the critical pressure ratio. In this context, the term critical
refers to the choked condition of the nozzle, at which the flow reaches sonic velocities at the throat of the nozzle.

\[ r_c = \left( \frac{2}{\gamma+1} \right)^{\gamma/(\gamma-1)} \]  

(2.6)

\[ K_N = \sqrt{\gamma \left( \frac{2}{\gamma+1} \right)^{\gamma+1} \frac{\gamma}{\gamma-1}} \]  

(2.7)

\[ v_{inj,c} = \frac{K_N}{r_c} \sqrt{\frac{p_0}{\rho_0}} \]  

(2.8)

\[ \dot{m} = C_d K_N A \sqrt{P_0 \rho_0} \]  

(2.9)

It should be noted that the specific heats at constant pressure and constant volume differ greatly with temperature and to a lesser degree pressure. However, since only the ratio of the specific heat ratio is used in this formulation, pressure effects are effectively negligible. Since the injection temperature remains within the low temperature regime, the assumption of constant specific heat ratios remains valid.

The only remaining unknown is the discharge coefficient \( C_d \).

\[ C_d = \frac{1}{2f r_c^{\frac{1}{\gamma}}} \left[ \left\{ 1 + \left( \frac{r_c-r \rho_c}{K_N^2} \right)^{\frac{1}{\gamma}} \right\} - \left\{ \left( 1 + \left( \frac{r_c-r \rho_c}{K_N^2} \right)^{\frac{1}{\gamma}} \right)^{2+} - \left( \frac{r_c^{\frac{1}{\gamma}}}{2r_c^{\frac{1}{\gamma}}} \frac{1}{1-(r_c-r \rho_c)} \right) \right\} \right] \]  

(2.10)
It should be pointed out that the expression for the discharge coefficient presented by Jobson includes a typographical error. The corrected equation is provided here, where the originally omitted power 2 is highlighted by arrows.

Jobson introduced a compressible correction to be applied to a previously determined incompressible discharge coefficient, $C_{d,i}$, by calculating the force defect arising from the increase of kinetic energy at the expense of pressure energy as the flow exits the nozzle. The force defect enters the expression for the discharge coefficient in the form of a force defect coefficient, $f_i$, which is related to the incompressible discharge coefficient $C_{d,i}$.

$$f_i = \frac{1}{C_{d,i}} - \frac{1}{2C_{d,i}^2} \quad (2.11)$$

This force defect results from a non-uniform pressure distribution at the nozzle exit. This reduced pressure at the nozzle exit thus causes an increase in flow rate as the pressure difference across the nozzle is increased. For clarity, a visual representation of this force defect taken from Jobson [38] is shown in Figure 2-1.
The force defect, as derived by Jobson, assumes that the compressible effects only take place at the nozzle and do not propagate upstream of the nozzle. The flow upstream of the nozzle is thus treated as incompressible. Bragg [39] pointed out that this leads to unrealistic results if the incompressible discharge coefficient is larger than 0.7. Accounting for the compressibility effects upstream of the nozzle, Bragg introduced the Modified Jobson’s Method, which calculates a compressible correction to the force defect coefficient.

Figure 2-1: Visualization of the Force Defect described by Jobson [38]

a For subcritical conditions.

b For supercritical conditions.
As the equations of the Modified Jobson’s Method cannot be closed explicitly, iterative methods must be utilized to solve the equations to determine the compressible discharge coefficient. It was found that using such iterative methods was in some cases sensitive to the initial guess made for $C_d$, especially when the first guess was taken as unity or close to unity. However, the incompressible discharge coefficient provided a convenient first guess that was suitable for the entire range of pressure ratios investigated here.

For the subcritical case, the following three equations are solved iteratively. First, the discharge coefficient is guessed to find $r_n$, which represents the pressure ratio of a hypothetical condition at the edge of the nozzle plane, and used to further calculate the compressible force defect coefficient and finally the compressible discharge coefficient.

\[
\frac{2}{r_n^\gamma (1 - r_n^{\gamma - 1})} = k^2 C_d^2 r_n^\gamma \left(1 - r_n^{\gamma - 1}\right) \tag{2.11}
\]

\[
f = \frac{2}{f_i} - \frac{(\gamma - 1)(1 - r_n)}{\gamma r_n^{2/\gamma} (1 - r_n^{\gamma - 1/\gamma})} \tag{2.12}
\]

\[
C_d = \sqrt{\frac{1 - \frac{2f(\gamma - 1)(1 - r_a)}{\gamma(1 - r_a^{\gamma - 1/\gamma})}}{2f_i^{2/\gamma}}} \tag{2.13}
\]

The supercritical case is solved analogously, except that the nozzle pressure ratio, $r_a$ is replaced by the critical pressure ratio.

\[
\frac{2}{r_n^\gamma (1 - r_n^{\gamma - 1})} = k^2 C_d^2 r_n^\gamma \left(1 - r_c^{\gamma - 1}\right) \tag{2.14}
\]

\[
r_c = \left(\frac{2}{\gamma + 1}\right)^{\gamma - 1} \tag{2.15}
\]
\[
\frac{f}{f_i} = \frac{2}{r_n^{1/y}} - \frac{(y-1)(1-r_n)}{y r_a^{2/y} (1-\frac{y-1}{y})} 
\]
(2.16)

\[
C_a = \frac{1+rc-ra}{rr_c} \sqrt{\left(1+\frac{rc-ra}{rr_c}\right)^2 - 2f_i^2 \frac{y}{r} (1-ra)} 
\]
(2.17)

The constant \( k \) in this model represents a geometry dependent factor for each flow nozzle that is otherwise uninfluenced by location within the nozzle nor by the flow conditions, and can thus be viewed as the geometry-only dependent part of the discharge coefficient. For Borda-Mouth Pieces \( k=0 \), and for smooth converging nozzles \( k=1 \), in the limiting extreme cases. For the incompressible case with constant incompressible discharge coefficient, Bragg related this parameter, \( k \), to the incompressible force defect coefficient such that \( k^2=2f_i \), where \( f_i \) is a function of \( C_{di} \). However, in this model, the incompressible discharge coefficient is taken to be variable and dependent on Reynold’s Number. For that reason, \( k \) is treated as a simple input variable to the model that requires experimental validation with each nozzle geometry modelled. It is taken as unity for comparability of the results presented below.

### 2.2.2. Incompressible Discharge Coefficient

Similar to the compressible discharge coefficient, which varies with flow conditions, so does the incompressible discharge coefficient vary. While treating the discharge coefficient as a constant is common practice for manual calculations over a limited range of flow conditions, the variations become significant if the range of flow conditions is wide.
Despite the difficulties in comparing discharge coefficients due to the strong influences of
the specific nozzle or orifice geometry, numerous empirical relationships have been
proposed to predict discharge coefficients. Most commonly, such empirical expressions are
functions of Reynold’s Number. Additionally, geometric factors, such as the ratio of throat
to pipe diameter, as presented in the model by Miller [40]. Quing et. al. further present
multiple expressions for the discharge coefficient for both subcritical and critical flows, and
relations for the effects of length-to-width ratio and recess ratio of the injector [41].

Especially at low Reynold’s numbers, it can be seen that the discharge coefficient
significantly drops compared to the relatively constant behavior as Reynold’s Numbers
become large. Micklow et. al. [37] presented two such empirical relationships for the
discharge coefficient of cylindrical and conical nozzles for incompressible flow that are
purely dependent of Reynold’s Number.

For Cylindrical Nozzles: \( C_{d,i} = 0.91 - 8.49/Re^{0.5} \)  \hspace{1cm} (18a)

For Conical Nozzles: \( C_{d,i} = 0.96 - 10.17/Re^{0.5} \)  \hspace{1cm} (18b)

For this model, the expression for conical nozzles by Micklow et. al. is utilized to determine
the incompressible discharge coefficient and provide closure to the Modified Jobson’s
Method. This relatively simplistic model only dependent on Reynold’s number was chosen
to minimize the number of tuning constants present in the overall model, leaving the
dependent geometric factor, \( k \), as the only input variable to the nozzle geometry.
2.2.3. Compressibility Effect on Viscosity

Since the incompressible discharge coefficient is a function of Reynold’s number, which in turns requires knowledge of the viscosity, an empirical model was used to define the viscosity of the injection gases at the various injection temperatures and pressure. While viscosity is primarily a function of temperature, at very high pressures viscosity becomes dependent on pressure as well.

At moderate pressures, the viscosity of hydrogen is dependent only on temperature. For any automotive direct injection process, the reduced temperature range is expected to be $5 \leq T_R \leq 75$. Stiel et. al. [42] found the following empirical relationship, where $\mu^*$ is the temperature dependent viscosity in centipoise at moderate pressures. The reduced quantities for temperature, pressure and density are defined as:

$$\mu^*(T) = 208 \times 10^{-5} T_R^{0.65} \quad (2.19)$$

$$T_R = \frac{T}{T_c} \quad \text{where } T_c = 33.3 \ K \quad (2.20)$$

$$P_R = \frac{P}{P_c} \quad \text{where } P_c = 12.8 \ atm \quad (2.21)$$

$$\rho_R = \frac{\rho}{\rho_c} \quad \text{where } \rho_c = 0.0310 \ g/cm^3 \quad (2.22)$$

For high pressures, Stiel presents data for a pressure correction to the solely temperature dependent expression in the form of a differential viscosity, $\Delta \mu(\rho_R) = \mu(T,P) - \mu^*(T_R)$, but unfortunately does not provide any empirical relationship for the presented data and curve fit. This data was used to develop an empirical expression for $\Delta \mu(\rho_R)$. 

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For $0 \leq \rho_R \leq 1.5$ the differential viscosity is estimated as

$$\Delta \mu(\rho_R) = 17.859 \times (e^{1.8986\rho_R} - 1)$$  \hspace{1cm} (2.22)$$

and for $\rho_R > 1.5$, the following 6th order polynomial expression was found, such that $\mu(T, P) = \mu^*(T) + \Delta \mu(\rho_R)$ gives the temperature and pressure dependent viscosity in centipoise.

$$\Delta \mu(\rho_R) = \{3000.5 \times \rho_R^6 - 27097 \times \rho_R^5 + 99144 \times \rho_R^4 - 186538 \times \rho_R^3 + 188556 \times \rho_R^2 - 95545 \times \rho_R + 18604\} \times 10^{-5}$$ \hspace{1cm} (2.23)$$

These expressions were found through regression analysis and are accurate within the readability limits of the data presented by Stiel, as represented in Figure 2-2.

![Differential Viscosity Regression](image)

**Figure 2-2: Pressure-dependent differential viscosity regression**
The reservoir total pressure, $P_0$, and reservoir total temperature, $T_0$, are set as input variables to the combined model, allowing for the calculation of the reservoir density, $\rho_0$. In many cases, gaseous injectors are designed to operate at choked conditions in order to provide a constant injection profile. For normally aspirated compression ignition engines with compression ratios on the order of 15-20, where the injection event occurs prior to the pressure rise due to combustion, this means that the injection pressure must be on the order of 30-40 atm in order to maintain the choked flow. Within this pressure range, it can be seen that viscosity increases nearly linearly with pressure, while $\mu^*$ remains constant, since the injection temperature is held constant at 300 K. As shown in Figure 2-3, pressure effects on dynamic viscosity are mostly negligible, accounting only for about 0.5% of the value of
dynamic viscosity. The pressure correction for viscosity was, however, still implemented for flexibility of the presented model to be used for higher pressure applications, such as forced induction engines and cases where the injection event and combustion pressure rise overlap.

2.2.4. Compressibility Effect on Density

At these pressures on the order of 40 atm, real gas effects become significant such that the compressibility factor must be accounted for in the calculations. Numerous empirical models exist for various gases to predict the compressibility factor, Z. The compressibility factor is commonly found in many fluid dynamics textbooks in the form of generalized plots as a function of reduced temperature and pressure, i.e. the ratio of actual temperature and pressure over their respective critical point values. While these plots provide a convenient method for hand calculations, they do not lend themselves to be easily implemented in computer code. Alternatively, generalized algebraic expressions applicable to various substances exist, which are much more easily implemented in computer codes. The Redlich-Kwong model [43], the Peng-Robinson model [44] and the Lee Kesler model [45] are among the most well-known such models. In this model, an expression specifically applicable to hydrogen was implemented. The model, which was proposed by Lemmon et. al. [46] was utilized here for its simple implementation, which does not require iterative processes, and its high accuracy of 0.01% error within the pressure and temperature ranges expected for gaseous fuel direct injection into CI engines.
\[ Z(P, T) = \frac{p}{\rho RT} = 1 + \sum_{i=1}^{9} \left\{ a_i \left( \frac{100K}{T} \right)^{b_i} \left( \frac{p}{1\text{MPa}} \right)^{c_i} \right\} \]  

(2.24)

**Table 2-1: Compressibility Model Coefficients**

<table>
<thead>
<tr>
<th>( i )</th>
<th>( a_i )</th>
<th>( b_i )</th>
<th>( c_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.058 884 60</td>
<td>1.325</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>-0.061 361 11</td>
<td>1.870</td>
<td>1.00</td>
</tr>
<tr>
<td>3</td>
<td>-0.002 650 473</td>
<td>2.500</td>
<td>2.00</td>
</tr>
<tr>
<td>4</td>
<td>0.002 731 125</td>
<td>2.800</td>
<td>2.00</td>
</tr>
<tr>
<td>5</td>
<td>0.001 802 374</td>
<td>2.938</td>
<td>2.42</td>
</tr>
<tr>
<td>6</td>
<td>-0.001 150 707</td>
<td>3.130</td>
<td>2.63</td>
</tr>
<tr>
<td>7</td>
<td>0.958 852 8 \times 10^{-4}</td>
<td>3.370</td>
<td>3.00</td>
</tr>
<tr>
<td>8</td>
<td>-0.110 904 0 \times 10^{-6}</td>
<td>3.750</td>
<td>4.00</td>
</tr>
<tr>
<td>9</td>
<td>0.126 440 3 \times 10^{-9}</td>
<td>4.000</td>
<td>5.00</td>
</tr>
</tbody>
</table>

As expected, the compressibility factor depicted in Figure 2-4 is nearly proportional to pressure and changes only slightly more than linearly with increasing injection pressure at constant injection temperature, owing to the simplistic atomic structure of diatomic hydrogen. For hydrogen at 40 atm, the resulting decrease in density is nearly 10% compared to ideal gas calculations.
2.2.5. Implementation in KIVA-3V

The presented model was developed in MatLab to produce values for the injection velocity, mass flow rate and discharge coefficient over a wide range of pressure ratios. Finally, the complete model was implemented in KIVA-3V release 2, such that at each time step the average mass flow rate between the current time step, $t$, and the previous time step, $t-1$, was used to determine the mass to be introduced into the computational domain.

$$[tm]_{inj}^t = [tm]_{inj}^{t-1} + (\dot{m}^t + \dot{m}^{t-1}) \cdot dt/2$$  \hspace{1cm} (2.25)

The KIVA implementation was then back-checked against the MatLab model at various arbitrary pressure ratios to ensure proper functionality.
2.3. **Results**

All results presented in this section were obtained by implementing the combined models described above in MatLab and solving for injection pressures, $P_0$, ranging from 1 to 80 atm, while keeping the injection temperature, $T_0$, constant at 300 K and keeping the cylinder (i.e. receiving volume) pressure constant at 1 atm. The flow-independent geometry factor $k$ is taken to be unity for this comparison.

Figure 2-5 depicts the behavior of mass flow rate and injection velocity compared to the pressure ratio across the nozzle. It can be seen that injection velocity rises very quickly as the reservoir pressure is increased (i.e. the pressure ratio is decreased). As the nozzle gets choked at the critical pressure ratio, the velocity profile levels out. However, a slight positive slope remains due the effect compressibility on the density of the injection gas. If plotted directly versus the reservoir pressure, the mass flow rate displays a nearly entirely linear behavior with injection pressure. This is due to the fact that the mass flow rate is driven by the changes in density with increasing pressure. Thus, the density increases linearly even when the nozzle is choked, owing to the near linear behavior of compressibility factor, $Z$. 
Figure 2-5: Injection Velocity and mass flow rate vs pressure ratio

Figure 2-6 depicts the incompressible discharge coefficient and the compressibility-corrected discharge coefficient. As, expected the influence of the compressibility correction is small when the pressure ratio is near unity and increases as compressible effects become more prevalent when the difference in pressure is large. Notably, the incompressible discharge coefficient is quite low but rises quickly as pressure ratios depart from unity.
Discharge coefficients from various experimental studies are notoriously difficult to compare due to the strong dependence of discharge coefficient on even minute geometrical differences. Figure 2-7 compares the ratio of computed mass flow rate to ideal mass flow rate with literature results presented by Nagao et. al. [47] and depicted in Figure 2-8. The ideal mass flow rate here is computed identically to the analysis by Nagao (see equation 2.26). It should be noted that the computational results presented by Nagao only represent the effect of the compressibility factor $Z$ and does not incorporate additional compressible effects occurring inside the nozzle, such as the force defect described by Jobson, nor any
other real world effects, such as viscous contributions, which become significant at low Reynold’s Numbers. It is thus expected that the discharge coefficient presented by this model are overall lower, as these real flow contributions to the discharge coefficient are not addressed by these literature results.

\[ m_{\text{ideal}} = \frac{AP_0}{\sqrt{R_0/T_0}} \left\{ \gamma \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}} \right\}^{1/2} \]  \hspace{1cm} (2.26)

It was observed that the compressibility factor, \( Z \), has by far the most significant effect on the mass flow rate. The effect of viscosity, and especially viscosity variation with pressure, on the other hand is mostly insignificant. Further, the model presented here predicts a significantly steeper drop of discharge coefficient at low Reynold’s Number, which is due to the incorporation of the reduction of incompressible discharge coefficient at low Reynold’s Number. This sharp drop in discharge coefficient is similarly described by other publications of experimental investigations such as Moroika et. al. [48] and Belforte [49]. However, this low Reynold’s Number flow regime is expected to be rarely encountered in most internal combustion injection applications. The maximum value of discharge coefficient, occurring at Reynold’s Numbers around 10^5 matches the literature data well for the presented case of smooth converging nozzle with geometric tuning constant, \( k \), equal to unity. In cases where the nozzle significantly departs from the assumption of the smooth converging nozzle, this tuning constant provides a convenient method for adjustment to the model based on experimental data. The reduction in discharge coefficient with increasing Reynold’s Number due to compressibility effects of the reservoir gas is qualitatively well-
captured. Again, the introduction of additional compressibility effects near the nozzle reduce the quantitative values in this regime.

It should be noted, that the discharge coefficient, as defined in Figure 2-7 and Figure 2-8, includes the effect of the compressibility factor, while the discharge coefficient defined within the Modified Jobson’s Method does not include the compressibility factor as these effects are already incorporated in the density calculation for the model presented here.

Figure 2-7: Ratio of Computed mass flow rate to ideal mass flow rate
2.4. Conclusions

A comprehensive 1-D model to describe the injection mass flow rate and injection velocity of a compressible gas is presented. The model was implemented in KIVA 3V release 2 to predict these quantities for a fixed injection reservoir pressure into a volume with time-varying pressures. The compressible injection model was based on the analytically derived Jobson’s Method and extended to account for various compressibility effects.

The model incorporates the compressibility factor, $Z$, which for this model was implemented for hydrogen. The compressibility factor was shown to have significant effects on the
injection mass flow rate and velocity due to the 10% reduction in density for pressures of 40 atm.

An empirical expression for the pressure variation of hydrogen viscosity was developed and implemented. Viscous variations with pressure were found to be nearly negligible at a reservoir pressure of 40 atm and a reservoir temperature of 300 K.

The incompressible discharge coefficient was modelled similarly to a previously developed incompressible injection model and in particular describes the significant drop in flow rate at low Reynold’s Numbers due to the increasing significance of viscous effects in this flow regime.

The incompressible discharge coefficient is modified through application of the Modified Jobson’s Method to incorporate compressible pressure drops at the nozzle exit arising from the high jet exit velocity. The compressible correction to the discharge coefficient increases the discharge coefficient by roughly 10% in the choked flow regime while approaching zero as the pressure ratio approaches unity.

The peak discharge coefficient of about 0.98 occurs at Reynold’s Numbers of $10^5$ for the case of a smooth converging nozzle, which is on the same order as suggested by literature data for ideal nozzles. If the nozzle significantly departs from the smooth, slowly converging nozzle assumption, the flow-independent geometry factor, $k$, in the presented model provides a convenient tuning constant to account for specific nozzle geometries based on experimental data.
2.5. Nomenclature

2.5.1. Variables and constants

\( v_{inj} = \text{injection velocity} \)

\( P = \text{pressure} \)

\( T = \text{Temperature} \)

\( \dot{m} = \text{mdot} = \text{injection mass flow rate} \)

\( \rho = \text{density} \)

\( A = \text{nozzle area} \)

\( C_d = \text{discharge coefficient} \)

\( \gamma = \text{specific heat ratio} \)

\( r = \frac{P}{P_0} = \text{pressure ratio} \)

\( K_N = \text{mass flow coefficient} \)

\( f = \text{force defect coefficient} \)

\( \mu = \text{dynamic viscosity} \)

\( \Delta \mu = \text{differential viscosity to account for pressure effects on viscosity} \)

\( k = \) geometry dependent constant uninfluenced by location within the nozzle nor by the flow conditions

\( Re = \text{Reynold's Number} \)

\( tm_{inj}^t = \text{total mass injected between } t = 0 \text{ and current time step} \)

\( dt = \text{time step} \)

\( R = \text{universal gas constant} \)
2.5.2. Suffixes

\( c = \text{critical} \)

\( i = \text{incompressible} \)

\( 0 = \text{total reservoir quantity} \)

\( \text{liq} = \text{liquid} \)

\( \text{cyl} = \text{condition in cylinder/injection receiving volume} \)

\( n = \text{hypothetical condition at edge of orifice} \)

\( a = \text{flow conditions on expansion to atmospheric pressure} \)

\( R = \text{reduced} \)

\( t = \text{computational time level} t \)

\( * = \text{only temperature dependent at moderate pressures} \)
Chapter 3
Spray Particle Breakup Models

This chapter investigates the spray droplet breakup models for primary and secondary droplet breakup and implements the Cascade Atomization and Drop Breakup model to address the underprediction of droplet size by the Taylor Analogy Breakup model.

The contents of this chapter have previously been substantially published by this researcher under the title “Primary and Secondary Spray Breakup Modelling for Internal Combustion Engine Applications” in the Journal of Multidisciplinary Engineering Science and Technology (JMEST), Vol. 6 Issue 4, April - 2019, ISSN: 2458-9403. [50]

3.1. Introduction

Spray modelling and droplet breakup represent one of the most crucial steps in the simulation of direct injected internal combustion engines, as the macroscopic spray parameters, such as spray penetration and spreading angle, along with the droplet characteristics, especially particle size distribution, determine the spatial distribution of gaseous combustible fuel within the cylinder. Failure to correctly predict particle size distributions will lead to an incorrect prediction of the evaporation and the resulting gaseous fuel distribution, which will then lead to errors in the combustion process calculation. The difficulty in fully describing and modelling a spray jet and breakup processes is due the large number of highly interconnected phenomena and mechanisms, such as primary and secondary breakup, heat transfer, evaporation, particle-particle interactions, aerodynamic forces, fluid forces (e.g.
surface tension), droplet deformation etc. Failure to accurately describe any one of these mechanism may mask issues in the description of the other processes.

The particle breakup process is generally divided into two categories, i.e. the Primary Breakup and the Secondary Breakup. The primary breakup describes the transformation of the cylindrical liquid column emanating from the injector nozzle into distinct particles due to instabilities arising from the surface tension and forces introduced by the injector nozzle geometry, as well as due to aerodynamic effects. In most computational models that do not model the multiphase flow inside of the injector, such as Reynold’s-Averaged-Navier-Stokes (RANS) calculations, the primary breakup is assumed to take place instantaneously at the nozzle exit and the liquid column is not explicitly simulated. Advanced simulation techniques such as Large Eddy Simulations (LES) and Direct Numerical Simulation (DNS) are generally required to explicitly model the liquid column. This simplifying assumption stands in contrast to the liquid core observed in real world sprays, which is depicted in Figure 3-1.
Due to essentially the same processes as primary breakup, the secondary breakup describes the further breakup of the primary fuel particles into increasingly fine fuel mist. Both primary and secondary breakup occur in various modes, depending on the ambient and particle characteristics, as described by the non-dimensional quantities, i.e. Reynold’s Number, Weber Number and Ohnesorge Number. Reynold’s Number is the ratio of inertial to viscous forces and is generally used to as a measure of turbulence in flows. Weber number is the ratio of inertial to surface tension forces and is useful in describing the interface of multiphase flows. Ohnesorge Number relates viscous forces to both inertial and surface tension forces, and is used to describe free surface fluid dynamics.
As Weber Number increases, both primary and secondary breakup produce larger numbers of smaller particles. High Weber Number sprays are therefore of particular interest for engine direct injection systems, to ensure the quick and complete atomization and evaporation of the liquid fuel.

3.2. Primary Breakup

Many investigators simply set the initial drop radius equal to the radius of the nozzle exit [52]. This practice likely arose from the observation that the liquid core emanating from a nozzle is roughly the same diameter as the nozzle, which remains a common assumption in the derivation of jet core dynamics.

Depending on the nozzle exit conditions, the primary breakup exhibits various breakup modes. At low injection velocity, the jet falls within the Rayleigh Regime or varicose breakup regime, which describes dripping flows. Instabilities arising from surface tension effects dominate this regime, which is characterized by large liquid column lengths and low velocity vectors perpendicular to the spray axis, resulting in long primary breakup lengths and low spreading angles. The Rayleigh Regime is depicted in Figure 3-2a).
As depicted in Figure 3-3, the ligament first stretches until the diameter of the stretched ligament approaches zero, at which point breakup occurs and deformed particles are formed. Restoring surface tension forces then cause the particle to contract into a more spherical shape, which results in a particle that is larger than the originating nozzle and respective jet core ligament. Applying stability analysis according to Rayleigh [54] for the maximum growth rate of an axisymmetric disturbance and the corresponding wavelength and wave number leads to a spherical droplet diameter approximately 1.89 times larger than the nozzle diameter. However, Sunol et. al point out, that in experimental results, the droplets are often measured to be significantly larger (between two and three times the nozzle diameter) than
this theoretical value, which they confirmed with high-speed videography to be due to coalescence events occurring shortly after the initial breakup event [55].

Figure 3-3: Evolution of Ligament Stretching and Particle Formation with Satellite Particles [56]

Kerst et al. propose the following relationship between droplet Sauter mean diameter and nozzle diameter, which reverts to $1.88 \, d_{\text{nozzle}}$ if the Ohnesorge number is small [53].

$$r_{3,2} = 3r_n \left(\frac{3\pi}{\sqrt{2}}\right)^{\frac{1}{3}} (1 + 3 \, \text{Oh})^\frac{1}{6} \quad (3.1)$$

This regime exhibits very little (less than 5%) variation in droplet diameter [57]. As is commonly done, the variation in droplet diameter can thus often be neglected with minimal impact on accuracy.
The Wind-Induced Regime occurs at intermediate injection velocities and is often subdivided into the First Wind-Induced (FWI) or sinuous wave breakup regime, and the Second Wind-Induced (SWI) or wave-like breakup with air friction regime. The FWI regime is characterized by droplet diameters of the about same size as the nozzle exit. The common practice of setting the initial drop size equal to the nozzle is thus mostly applicable to this regime. In the FWI regime, surface tension is the main contributing source of instabilities and is opposed by inertia and air resistance, which results in surface waves and the production of ligaments, whose breakup is furthered by the air resistance.

In the SWI regime, as jet velocity and Weber number further increase, air resistance no longer acts as a damping factor but rather increases perturbations. Droplets in this regime are generally smaller than the nozzle diameter. Many empirical models exist to predict the droplet size in the wind induced regime, many of which are of similar format. Two such examples are the models by Harmon [58],

\[
d_{3,2} = 3330 \left( d_n^{0.3} \mu_l^{0.07} \rho_l^{-0.648} \sigma^{-0.15} u^{-0.55} \mu_g^{0.78} \rho_g^{-0.052} \right) \tag{3.2}
\]

and Wu et al. [59], [60]

\[
d_{3,2} = \frac{7 d_n}{W e_g} \left( \frac{x}{d_n \sqrt{R e_l}} \right)^{0.87} \tag{3.3}
\]

for 0.4 or 13 ≤ We_g < 40.3, where x is the axial distance from the nozzle.
The atomization regime, which occurs at high Weber numbers, is by far the least well understood regime. The liquid core dramatically changes in shape in the atomization regime, producing a conical structure rather than an elongated cylinder. Similar to stripping or catastrophic secondary breakup, relatively small droplets are stripped from the surface of the liquid cone through air friction effects, reducing the radius of the liquid cone with increasing distance from the nozzle, as shown in Figure 3-4. A great difficulty in experimental investigations of primary atomization arises from the limitations of current measurement techniques. Optical techniques, such as Schlieren photography, shadowgraphy and video/photography can only visualize the external structure of the spray and measure penetration distance and spreading angle of the spray. The internal spray structure, including the liquid core and droplet sizes, is obscured by the fine atomized spray at the outer edge of the spray. Other methods, such as X-Ray tomography can penetrate the optically dense outer spray, but many such techniques require a very small sampling volume and may require for only a single particle to be present within that volume in order to determine droplet size. The near-injector region, however, is characterized by a high droplet number density.

Figure 3-4: Sketch of Primary and Secondary Liquid Jet Breakup [61]
For the atomization regime, one of many semi-empirical formulations for the Sauter mean diameter of the particle, \( SMD \) or \( d_{3,2} \), may be utilized if the model does not inherently assume sphericity of particle. One such formulation was implemented in the KIVA code by Micklow et. al. [37], based on the experimental results by Elkotb [62].

\[
\frac{d_{3,2}}{d_n} = 109.52 \left( Re^{-0.183} We^{-0.442} C_d^{-0.442} \left( \frac{\rho_l}{\rho_a} \right)^{-0.05} \right)^{0.442}
\]  

(3.4)

for \( 40.3 \leq We_g \)

Figure 3-5 depicts the various primary breakup regimes as a function of Reynold’s Number and Ohnesorge Number, which is a dimensionless number relating the viscous forces to the inertial and surface tension forces. The figure also locates the two cases investigated in this paper, as well as roughly outlining the region of conditions applicable to common Diesel direct injection engines on the \( Re-Oh \) plot. Seeking cleaner combustion through improved atomization, injection pressures have drastically increased to the high and ultra-high injection pressure region over the last decades, meaning the conditions for such ultra-high pressure systems may lie further in the atomization regime on the \( Re-Oh \) plot. Reitz [63] further extended this \( Re-Oh \) plot to include the density ratio, \( \rho_g/\rho_l \), showing that increases in the density ratio increased breakup due to increased aerodynamic forces.
3.3. Secondary Breakup

Secondary breakup models describe the processes by which existing droplets break up to form smaller particles. Like the primary breakup, several breakup modes exist for secondary breakup. As Weber number increases, aerodynamic effects increase and facilitate faster breakup, resulting in the formation of increasingly smaller droplets with increasing Weber number. The various secondary breakup modes are depicted in Figure 3-6.
3.3.1. TAB Model

The Taylor Analogy Breakup (TAB) model developed by O’Rourke and Amsden [65] is the native model in the KIVA code set. The TAB model draws the analogy between a mass spring damper system and the oscillation of the distorting liquid droplets.
Starting with the general equation for a damped, forced oscillator

\[ F - kx - d \frac{dx}{dt} = m \frac{d^2x}{dt^2} \]  

(3.5)

with Taylor Analogy coefficients,

\[ \frac{F}{m} = C_F \frac{\rho g u^2}{\rho_l r} \]  

(3.6a)

\[ \frac{k}{m} = C_k \frac{\sigma}{\rho_l r^3} \]  

(3.6b)

\[ \frac{d}{m} = C_D \frac{\mu_l}{\rho_l r^2} \]  

(3.6c)

where the constants, \(C_k=8\), \(C_D=5\), and \(C_F=1/3\) are determined experimentally, the oscillator equation is non-dimensionalized assuming only a single mode of oscillation and setting \(y = \frac{x}{c_b r}\), leading to the following equation:

\[ \frac{d^2y}{dt^2} = \frac{C_F \rho g u^2}{c_b \rho_l r^2} - \frac{C_k \sigma}{\rho_l r^3} y - \frac{C_D \mu_l}{\rho_l r^2} \frac{dy}{dt} \]  

(3.7)

Further assuming underdamping of the droplets and constant relative velocities, the non-dimensional expression can be solved for the time rate of change of the distortion \(dy/dt\), as well as for the distortion, \(y\), where breakup occurs if \(y > l\). The general solutions to these equations are

\[ y(t) = W e_c + e^{-\frac{t}{t_d}} \left[ (y_0 - W e_c) \cos(\omega t) + \frac{1}{\omega} \left( \frac{d y_0}{dt} + \frac{y_0 - W e_c}{t_d} \right) \sin(\omega t) \right] \]  

(3.8)
and

\[
\frac{dy}{dt}(t) = \frac{W_{e_c} - y(t)}{t_d} + \omega e^{-\frac{t}{t_d}} \left\{ \frac{1}{\omega} \left( \frac{y_0 - W_{e_c}}{t_d} + \frac{dy_0}{dt} \right) \cos(\omega t) - (y_0 - W_{e_c}) \sin(\omega t) \right\}
\]

where the Weber number and critical Weber number are defined as

\[
We = \frac{\rho u^2 \gamma}{\sigma}
\]

\[
W_{e_c} = C_F C_k C_b We = \frac{We}{12}
\]

Further, the initial distortion and initial time rate of change of distortion are assumed to be zero at the point of injection.

\[
y_0 = y(0)
\]

\[
\frac{dy_0}{dt} = \frac{dy}{dt}(0)
\]

The drop time constant and oscillation frequency are given by

\[
t_d = \frac{2 \rho l \gamma^2}{c_D \mu_l}
\]

\[
\omega = \sqrt{\frac{C_k \sigma}{\rho l \gamma^2} - \frac{1}{t_d}}
\]
Solving the energy equation for the distorted child and parent droplets and equating the internal energy of the deformed parent droplet with the internal energy of all child droplets allows for the calculation of the child droplet size. As the child droplet is initially assumed not to be deformed in the TAB model, the Sauter mean radius is equivalent to the drop radius.

\[ r_{3,2,\text{child}} = \frac{r}{1 + \frac{8K}{20} \rho r^3 \left( \frac{dy}{dt} \right)^2 (\frac{6K-5}{120})} \quad (3.14) \]

The number of child droplets is found through conservation of mass.

\[ N^{n+1} = N^n \left( \frac{r^n}{r^{n+1}} \right)^3 \quad (3.15) \]

The child droplets further receive a velocity component normal to the parent droplet velocity, given by

\[ v_{\text{normal}} = C_v C_b \frac{dy}{dt} \text{ where } C_v \approx 1 \quad (3.16) \]

By finding the distortion amplitude, \( A \), and assuming that the first oscillation period is not damped, the breakup time becomes the smallest possible root of an undamped version of equation (8) that is larger than the current time \( t_n \).

\[ A = \sqrt{(y_n - W e_c)^2 + \left( \frac{dy}{dt} \right)^2} \quad (3.17) \]

\[ W e_c + A \cos [\omega(t - t^n) + \Phi] = 1 \quad (3.18) \]
The breakup criterion can thus be defined as

\[ We_c + A > 1 \]  \hspace{1cm} (3.19)

If breakup does not occur during the time step, the droplet distortion and rate of distortion are updated as follows:

\[ y^{n+1} = We_c + e^{-\frac{\Delta t}{t_d}} \left\{ (y^n - We_c) \cos(\omega t) - \frac{1}{\omega} \left[ \left( \frac{dy}{dt} \right)^n + y^n - We_c t_d \right] \sin(\omega t) \right\} \]  \hspace{1cm} (3.20)

\[ \left( \frac{dy}{dt} \right)^{n+1} = \frac{We_c - y^{n+1}}{t_d} + \omega e^{-\frac{\Delta t}{t_d}} \left\{ \frac{1}{\omega} \left[ \left( \frac{dy}{dt} \right)^n + y^n - We_c \right] \cos(\omega t) - (y^n - We_c) \sin(\omega t) \right\} \]  \hspace{1cm} (3.21)

where

\[ \cos(\Phi) = y^n - \frac{We_c}{A} \]

\[ \sin(\Phi) = -\frac{\left( \frac{dy}{dt} \right)^n}{A\omega} \]

The TAB model has been surrounded by controversy. As Lee [66] points out, the original TAB paper by O’Rourke and Amsden included a typographical error in the \( \sin(\omega t) \) part of the \( \frac{dy}{dt} \) equation (equation 3.9), switching \( y \) and \( \frac{dy}{dt} \) within the expression. However, it was verified that this error did not perpetuate into the KIVA source code, which was coded correctly. Lee et. al. further points out that the TAB model analysis of Ibrahim et. al. [67]
omitted a factor of 0.5 in its presentation, leading to the TAB results as being incorrectly represented. Nonetheless, the TAB model tends to over-predict the breakup process, leading to excessively small particles.

3.3.2. ETAB Model

The TAB model has been criticized for under-predicting droplet sizes and subsequently an entire class of breakup models has been developed based on a similar approach. The Enhanced Taylor Analogy Breakup (ETAB) model proposed by Tanner [68] marks the next step in the evolution of this model. The ETAB model utilizes largely the same algorithm, but with two notable modifications. The first difference is that in the ETAB model the production rate of child droplets is assumed to be proportional to the number of child droplets, where the proportionality constant is dependent on the breakup regime.

\[
\frac{dN}{dt}(t) = 3K_{br}N(t) \tag{3.22}
\]

\[
K_{br} = \begin{cases} 
\frac{k_1\omega}{k_2\omega\sqrt{We}} & \text{for } We \leq We_t \\
\frac{k_1\omega}{k_2\omega\sqrt{We}} & \text{for } We > We_t 
\end{cases} \tag{3.23}
\]

where

\[We_t=80\]

\[k_1=2/9 = \text{ETAB Bag Breakup Factor}\]

\[k_2=2/9 = \text{Stripping Breakup Factor}\]
The uniform droplet size distribution is then determined by

\[
\frac{r_{\text{child}}}{r_{\text{parent}}} = e^{-K_{br}t} \quad (3.24)
\]

The child particles are initialized with zero distortion and zero rate of distortion. Similar to the original TAB model, the child particles assume a velocity component perpendicular to the parent particle

\[
v_{\text{normal}} = A_c \frac{dx}{dt} \quad (3.25)
\]

Where \( A_c \) is a constant describing how much of the axial parent velocity is converted to a normal velocity for the child particle and is determined from energy balance considerations.

\[
A_c = \sqrt{3 \left[ 1 - \frac{r_{\text{parent}}}{r_{\text{child}}} + \frac{5C_D We}{72} \right] \left( \frac{\omega}{\frac{dy}{dt}} \right)} \quad (3.26)
\]

Where \( C_D \) is the drag coefficient and the distortion frequency, \( \omega \), is given by

\[
\omega = \sqrt{\frac{C_k \sigma}{\rho \ell r_{\text{parent}}}} \quad (3.27)
\]

However, unlike the standard TAB model, this normal velocity is now variable such that the normal velocity increases with increasing Weber number. The second major difference is that the ETAB model no longer assumes that the rate of droplet distortion \( \frac{dy}{dt} \) to be initially zero upon injection and breakup.
\[
\begin{align*}
\frac{dy}{dt}(0) &= \{1 - We_c[1 - \cos(\omega t_{bu})]\}\frac{\omega}{\sin(\omega t_{bu})} \\
t_{bu} &= C \sqrt{\frac{\rho_p d_{p,0}}{\rho_f v_{p,0}}} \text{ where } C = 5.5
\end{align*}
\]

3.3.3. CAB Model

In a further iteration of the TAB model, Tanner introduced the Cascade Atomization and Drop Breakup (CAB) model [69]. The CAB model expands on the ETAB model, utilizing the exact same methodology, except for a refinement of the breakup constant used to obtain child droplet sizes.

\[
K_{br} = \begin{cases} 
    k_1 \omega & 5 < We < 80 \\
    k_2 \omega \sqrt{We} & 80 < We < 350 \\
    k_3 \omega We^{3/4} & 350 < We
\end{cases}
\]

\[
k_2 = \frac{k_1}{\sqrt{1 - \frac{c_k c_b}{2 c_f Wet}}} \quad (3.30a)
\]

\[
k_3 = \frac{k_2}{We_t^{1/4}} \quad (3.30b)
\]

Where \( k_1 = 0.05, We_t = 80, We_t^2 = 350 \)
3.3.4. MCAB Model

Finally, Kumzerova [70] further extended the applicability of the CAB model for very high and very low Weber Numbers by further optimizing the breakup constants, naming this extension the Modified Cascade Breakup (MCAB) Model.

3.3.5. WAVE Model

Unlike the TAB model, the wave family of breakup models is derived from the stability analysis of cylindrical, viscous liquid jets into a gaseous, incompressible and inviscid gas. While the TAB model is limited to relatively low Weber numbers, the Wave model, developed by Reitz [52], is especially applicable to high speed injections with Weber numbers above 100. The Wave model assumes a liquid injection core, which is subjected to a relative velocity between the liquid and gas phase, resulting in Kelvin-Helmholtz instabilities as a result of aerodynamic effects.

3.3.6. KH-RT Model

The KH-RT represents a hybrid model proposed by Beale and Reitz [71] represents a further extension of the Wave model. As in the Wave model, the liquid core is subject to Kelvin-Helmholtz instability, describing the primary breakup of the jet. However, outside of the core, Rayleigh-Taylor breakup, which describes the instabilities on the droplet surface due to sudden acceleration of the ejected droplets into the freestream, becomes dominant.

3.3.7. SSD Model

All of the primary and secondary breakup models described above assume uniform initial droplet sizes due to the assumption of unimodal breakup. In real-world sprays, primary break
up results in both major and satellite particles as shown in Figure 3-3 and Figure 3-7b). A much more rigorous, but also more computationally expensive, approach to describe primary breakup with satellite formation was presented by Olesen [72].

For secondary breakup models, the Stochastic Secondary Droplet (SSD) model provides one alternative for modelling the multiple droplet size scales created by bimodal breakup and satellite formation [73]. The motivation for modelling these satellite particles has mainly been driven by the attempt to better predict gaseous fuel distributions especially near the injector nozzle by inclusion of these very small and quickly evaporating satellite droplets. However, Olesen found that satellite droplets only make up about 1.4% of the total spray mass owing to their relatively much smaller size, despite occurring in similar numbers as the main particles [72].

![Figure 3-7: a) idealized primary breakup b) real primary breakup with satellite droplet formation [74]](image)

Chryssakis et. al. provide a useful in-depth summary of these and other secondary breakup models [75].
3.4. Computational Model

For the work presented here, the ETAB and CAB secondary breakup models were implemented according to the equations outlined above and compared to the standard TAB model. Additionally, the effect of the primary breakup model on the results was investigated. To this end and for completeness, a primary breakup model based on the relations by Kerst (eqn. 3.1) for the Rayleigh regime, and on Wu et. al. (eqn. 3.3) for the Wind-Induced Regime was implemented. For the atomization regime, three primary breakup models were investigated, which are outlined in Table 3-1.

The model designated as PBU3, is a hybrid model of the Micklow/Elkotb model applied in the outer regions of the spray plume, and larger initial droplets at the center of the spray cone. This is accomplished by introducing a tuning constant, \(0 \leq k_\Psi \leq 1\), which determines the ratio of the spray angle for the core, \(\Psi_c\), and total spray angle, \(\Psi_{sp}\). Additionally, the droplet radius of the core region is reduced, as part of the liquid core has been abraded due to the atomization taking place at the outer edge of the liquid core. This reduction factor in this study is set equal to the same tuning constant, \(k_\Psi\). Since the spray at the beginning of the injection event encounters a stagnant ambient gas and the velocity profile near the injector due to momentum transfer to the gas and air entrainment has not yet been established, the entire spray cone experiences conditions that promote atomization. For this reason, a time offset for the initiation of the primary breakup reduction, estimated at 0.1 ms for this study, is introduced. Therefore, the expression \(d_{32} = 3k_\Psi d_n\) for \(\Psi < \Psi_c\) is only utilized 0.1 ms after the initiation of the injection event. The factor 3 in these models is due to the definition of the Sauter mean radius for a spherical particle, which states that the average radius \(\bar{r} = 1/3\)
PBU1 is thus an expression for setting the initial droplet radius equal to the injector nozzle radius.

Table 3-1: Primary Breakup (PBU) Models

<table>
<thead>
<tr>
<th>PBU</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBU1</td>
<td>( d_{3,2} = 3d_n )</td>
</tr>
<tr>
<td>PBU2</td>
<td>Micklow/Elkotb Model (eqn. 3.4)</td>
</tr>
</tbody>
</table>
| PBU3     | \( \begin{cases} 
                       d_{3,2} = 3kd_n & \text{for } \Psi < \Psi_c \\
                       \text{Micklow/Elkotb Model for } \Psi \geq \Psi_c \\
                       \text{where } \Psi_c = k\Psi_{sp} 
                       \end{cases} \) |

The primary breakup regimes were determined by the critical Ohnesorge Number lines presented in the \( Re-Oh \) plot, which are depicted in Figure 3-5 and represent the following power law functions.

\[
Reynold's \text{ Regime } \leq Oh_{c1}
\]

\[
Oh_{c1} < \text{Wind Induced Regime } \leq Oh_{c2}
\]

\[
Oh_{c2} < \text{Atomization Regime}
\]

Where

\[
Oh_{c1} = 50 \times Re^{-1.31} \quad (3.31a)
\]

\[
Oh_{c2} = 1587 \times Re^{-1.31} \quad (3.31b)
\]
For this study, the results were compared to two literature cases. The first case is a high ambient pressure, high ambient temperature, evaporating spray, presented by Naber and Siebers [76], which provides additional documentation and materials on the case presented on the Engine Combustion Network (ECN) website [77]. All simulations for this case were performed with a square mesh of 8x8x10.9 cm with 40x40x100 vertices and all solid wall boundary conditions. The test conditions are outlined in Table 3-2 and Table 3-3 below.

<table>
<thead>
<tr>
<th>Species</th>
<th>% Vol</th>
<th>% Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>N₂</td>
<td>90.33</td>
<td>88.37</td>
</tr>
<tr>
<td>CO₂</td>
<td>6.11</td>
<td>9.39</td>
</tr>
<tr>
<td>H₂O</td>
<td>3.56</td>
<td>2.24</td>
</tr>
</tbody>
</table>

Table 3-2: Gas Composition For Evaporative Case (Naber & Siebers)

<table>
<thead>
<tr>
<th>ΔP</th>
<th>139 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{amb}$</td>
<td>8.304 MPa</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>1000 K</td>
</tr>
<tr>
<td>$\rho_{amb}$</td>
<td>28.6 kg/m$^3$</td>
</tr>
<tr>
<td>$\Delta t_{inj}$</td>
<td>3.6 ms</td>
</tr>
<tr>
<td>$T_{inj}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$d_n$</td>
<td>0.198 mm</td>
</tr>
<tr>
<td>$V_{inj}$</td>
<td>308 m/s</td>
</tr>
<tr>
<td>$m_{inj}$</td>
<td>8 g/s</td>
</tr>
<tr>
<td>$d_{vol}$</td>
<td>109 mm</td>
</tr>
</tbody>
</table>

The second case represents a low ambient pressure, low ambient temperature, non-evaporating case in ambient air by Lee and Park [78].
The mesh for this case was a square mesh of 8x8x10 cm and 40x40x100 vertices, with an open boundary condition at the side opposite the injector and is depicted in Figure 3-8. In both cases the mesh size was chosen to recreate the experimental distance between the injector nozzle and the opposing wall, while avoiding wall effects and interactions on the mesh sides.

### Table 3-4: Test Conditions For Non-Evaporative Case (Lee & Park)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{amb}$</td>
<td>1 atm</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$P_{inj}$</td>
<td>80 MPa</td>
</tr>
<tr>
<td>$\Delta t_{inj}$</td>
<td>1.4 ms</td>
</tr>
<tr>
<td>$T_{inj}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$d_n$</td>
<td>0.3 mm</td>
</tr>
<tr>
<td>$\dot{m}_{inj}$</td>
<td>14.379 g/s</td>
</tr>
<tr>
<td>$V_{inj}$</td>
<td>266.24 m/s</td>
</tr>
<tr>
<td>$\psi_{sp}$</td>
<td>15.1 deg</td>
</tr>
</tbody>
</table>

In both cases, Diesel Fuel 2 (DF2) was utilized as the injection medium and injected via square injection pulses.
3.5. Results

Figure 3-13 depicts the spray evolution with time of the evaporating jet simulating the experimental conditions by Naber and Siebers. All models displayed here use the same primary breakup mechanism, PBU1, setting the initial droplet size equal to the injector nozzle diameter. The experimental results are shown in the first column. It must be emphasized here that Naber and Siebers explicitly state that in these experimental pictures full extinction of background light is associated with the extend of the liquid spray, while Schlieren effects or partial extinction of the background light is mainly associated with gaseous fuel and temperature gradients. Unfortunately, this makes the analysis of these pictures rather subjective, as the exact extend of the liquid spray is not readily determinable. For higher resolution pictures of the experiment, the reader is referred to the evaporating
case of the “Evaporating vs. Non-Evaporating” study by Naber and Siebers available through the Engine Combustion Network (ECN) [30]. It should further be noted that each particle marker in the simulations depicts a parcel representing multiple droplets.

The ETAB and CAB model (second and third column of Figure 3-13) perform with no discernable differences with respect to spray penetration and spray angle. In both cases, the spray characteristics appear well matched for the first 0.7 ms. After 1.26 ms, the spray angle notably exceeds the experimental results, and after 2.24 ms, the spray penetration of the models markedly enters the Schlieren region of the experimental photographs.

The TAB model (Figure 3-13 column 4) does not perform well under the modelled high ambient density conditions. Overprediction of breakup is the well-established main criticism on the performance of the standard TAB model. In the presented case, the high ambient density facilitates breakup and the high temperature evaporates the resulting small droplets nearly instantaneously such that a liquid spray plume is never developed.

For comparison, the last column of Figure 3-13 depicts the same simulation without secondary breakup mechanism, such that droplet size reductions are mainly due to evaporation. As expected, the jet penetration is overpredicted at all time steps. The spray angle, however, is well-matched, as no velocity gradients perpendicular to the droplet path are introduced by breakup processes in this case.

The non-evaporating case depicted in Figure 3-15 shows similar results to the evaporating case. Both the ETAB and CAB model again present with no discernable differences, but show slight over-predictions in spray penetration at 0.2 ms and 1.4 ms. While the TAB model
performs significantly better in this case, spray penetration is notably underpredicted, especially at the late stages of the spray development. Additionally, the low parcel density suggests that many droplets reached a lower cutoff size, at which the KIVA code converts these exceedingly small particles to the gas phase. Again, by inhibiting secondary breakup, the penetration distance is significantly overpredicted.

These results suggest that the CAB and ETAB model performance is significantly superior to the TAB model. However, the penetration distance and spray angle over prediction further suggest that the primary breakup model PBU1 overestimates the initial droplet size. This is further supported by the large droplet sizes relative to the nozzle diameter, especially near the spray tip, as depicted by the color bars in these figures. As shown in Figure 3-5, both cases are clearly located within the primary atomization regime. PBU1, however, is mostly applicable to the wind-induced regime. PBU2 (Micklow/Elkotb model) on the other hand is a primary atomization regime model.

The second and third columns of Figure 3-14 and Figure 3-16 compare the performance of primary breakup models PBU1 and PBU2 in conjunction with the CAB secondary breakup model. PBU1 matches the initial plume formation relatively well, but over predicts penetration and spray angle as the spray plume evolves. PBU2 significantly under-predicts spray penetration and spray angle in every plume development stage. These results led to the development of the hybrid model PBU3, depicted in the fourth column of Figure 3-14 and Figure 3-16. As already noted by Reitz [63], the primary breakup regime limits depicted in Figure 3-5 demark the onset of e.g. the atomization regime transition. However, the Micklow/Elkotb model (PBU2) assumes full atomization of the spray through primary
breakup alone. It is proposed that a significant transition regime between the wind-induced regime and the atomization regime exists, in which the outside of the spray cone experiences atomization, while the inner spray cone remains within the wind breakup regime, such that the extent to which atomization occurs increases with increasing Weber number. This bimodal behavior is due to the high aerodynamic shear forces at the outside of the jet causing atomization, while momentum transfer, air entrainment and particle-particle interactions significantly reduce the relative velocity between the gaseous medium and the droplets at the center of the spray cone. Thus, primary breakup is inhibited at the center of the jet. However, the resolution of most practical RANS simulation is too coarse to fully resolve these velocity gradients and particle interactions. An empirical formulation is therefore required to determine the ratio of spray within the atomization and wind-induced regime, respectively. As a first starting point, the PBU3 model utilizes a tuning constant, $k_{\Phi}$, to determine the ratio of the large particle core spray angle to the full spray angle, as well as the initial droplet size at the jet center. For comparability, all PBU3 simulations presented here are performed with $k_{\Phi}$ set to 0.5, meaning that the droplets originating from within one half of the full spray angle are assumed to be in the wind-induced regime.

Column 4 of both Figure 3-14 and Figure 3-16 show an improvement of the spray angle compared to the PBU1 and PBU2 CAB simulations, as well as an improvement of the spray penetration prediction for the well-developed spray. However, the spray penetration is still notably underpredicted at the early spray development stage.

It should be emphasized here that the initial droplet size at the core region, set to equal the nozzle radius, is only utilized to demonstrate the new bimodal primary breakup approach
and likely represents a significant over-estimation of the droplet size. Experimental research into the radial droplet size distribution is required to complete and validate the PBU3 bimodal approach. Similarly, the \( k_\Phi \) value of 0.5 was chosen empirically to fit the results presented here. Again, experimental data is still needed to determine an empirical relationship for this tuning constant as a function of spray conditions, as well as the initial time offset for the primary breakup reduction.

Figure 3-14 further depicts the performance of the primary breakup models without secondary breakup for comparison. Finally, Figure 3-16 presents the PBU2/TAB case for comparison, which again underpredicts spray penetration and spray angle due to extreme droplet breakup. The low spray angle and low parcel density, along with the small droplet radius depicted by the marker coloring support the conclusion that breakup is overpredicted.

The macroscopic spray characteristics, such as spray penetration and spray angle provide only a partial picture. Additional insight can be gained by examining the droplet size distributions. Figure 3-9 depicts the experimental axial droplet size distribution by Lee and Park, along with the parcel sizes predicted by the PBU3/TAB model. This figure demonstrates the extend of droplet size under-prediction by the TAB model, as most of the parcels are less than 1 micrometer in diameter, i.e. more than one order of magnitude less than the experimental average, and no parcels are predicted to be larger than the experimental average.
Figure 3-9: Droplet Size Distribution PBU3/TAB

Figure 3-10 depicts the same information for the PBU3/CAB model, with Figure 3-11 providing a magnification of the lower diameter range. In this case, the majority of parcels is in the 0 to 10 micrometer range, but are significantly more evenly distributed across this range than in the TAB model. A number of droplets are predicted at significantly larger diameters. These mainly correspond to droplets originating from the core region of the PBU3 model. The large predicted diameter of these parcels is partially due to coalescence through collision events, as well as overpredictions from the Gaussian distribution applied to the initial size distribution by KIVA [14]. These results further suggest that the initial droplet diameter in the core region, set to one half (in the presented case) of the nozzle diameter in the PBU3 model, represents an over-estimation and needs to be refined in future research based on experimental findings.
Figure 3-10: Droplet Size Distribution PBU3/CAB

Figure 3-11: Droplet Size Distribution PBU3/CAB (magnified)
Figure 3-12 shows that by neglecting to account for the reduced primary breakup at the core, the average droplet size is underpredicted, especially as the distance to the nozzle increases, as nearly all parcels are smaller than the average droplet size measured by Lee and Park. This further suggests that the jet does not completely atomize through the primary breakup alone and that primary breakup is in fact reduced at the center of the jet.

**Figure 3-12: Droplet Size Distribution PBU2/CAB**
Figure 3-13: Secondary Breakup Models for Evaporating Case (Naber & Siebers) 
(all cases utilizing PBU1)
Figure 3-14: Primary Breakup Models for Evaporating Case (Naber & Siebers)
Figure 3-15: Secondary Breakup Models for Non-Evaporating Case (Lee & Park) (all cases utilizing PBU1)
Figure 3-16: Primary Breakup Models for Non-Evaporating Case (Lee & Park)
3.6. Conclusions

The Enhanced Taylor Analogy Breakup (ETAB) and Cascade Atomization Breakup (CAB) model were implemented in KIVA 3V release 2 and results using these models were compared to the standard TAB model, as well as to two literature cases representing both evaporating and non-evaporating conditions within the atomization regime representative of Diesel direct injection conditions.

It was found that under the investigated conditions the ETAB and CAB model performed nearly identically, but represented a significant improvement compared to the TAB model with respect to predicting the spray penetration, spreading angle, droplet size and overall spray plume shape.

A comprehensive primary breakup model was implemented covering all primary breakup regimes. For the atomization regime a hybrid bimodal primary breakup mechanism was introduced to account for the reduced primary breakup due to the induced gas velocity, air entrainment and particle-particle interactions at the center of jet.

This bimodal approach showed improved performance of the model with respect to penetration distance, spray angle and droplet size, compared to the primary breakup model that assumes full atomization by primary breakup alone.

It should be noted that the bimodal primary breakup approach introduced here in its current stage is not meant to be seen as complete. Experimental data is still needed to describe the tuning constant used to determine the primary breakup reduction and droplet size at the spray center as a function of spray characteristics.
3.7. Nomenclature

3.7.1. Variables and Constants

\[ Re_l = \text{Reynold's Number} = \frac{u_{rel} d_{smr} \rho_l}{\mu_l} \]
\[ We_l = \text{Weber Number} = \frac{u_{rel}^2 d \rho_l}{\sigma} = \frac{\text{interial/aerodynamic forces}}{\text{surface tension}} \]
\[ Oh = \text{Ohnesorge Number} = \frac{\sqrt{We_l}}{Re_l} \]

\( \rho = \text{density} \)
\( \mu = \text{viscosity} \)
\( \sigma = \text{surface tension} \)
\( \Psi_{sp} = \text{total spray angle} \)
\( \Psi = \text{spray angle of individual parcel} \)
\( \omega = \text{distortion wave frequency} \)
\( A = \text{distortion amplitude} \)
\( A_c = \text{ratio of axial to normal velocity} \)
\( C = \text{constant (various)} \)
\( C_b = \text{critical amplitude coefficient} = 0.5 \)
\( C_a = \text{discharge coefficient} \)
\( C_0 = \text{damping coefficient} = 5.0 \)
\( C_f = \text{external force coefficient} = 1/3 \)
\( C_k = \text{restoring force coefficient} = 8.0 \)
\( C_v = \text{new droplet velocity factor} \)
\( d = \text{diameter} \)
\( F = \text{force} \)
\( K = \text{energy ratio factor} = 10/3 \)
\[ m = \text{mass} \]
\[ N = \text{number of droplets} \]
\[ P = \text{Pressure} \]
\[ r = \text{radius} \]
\[ T = \text{Temperature} \]
\[ dt = \text{time step} = t_2 - t_1 \]
\[ t = \text{time} \]
\[ td = \text{time constant} \]
\[ u = \text{velocity} \]
\[ V_{\text{inj}} = \text{injection velocity at nozzle} \]
\[ v_{\text{normal}} = \text{droplet normal velocity component} \]
\[ x = \text{distance} \]
\[ y = \text{distortion} \]

3.7.2. Sub/Superscripts

\[ 0 = \text{initial (} t = 0 \text{)} \]
\[ 3,2 = \text{Sauter Mean (radius or diameter)} \]
\[ c = \text{critical} \]
\[ d = \text{droplet} \]
\[ g = \text{amb = ambient gas} \]
\[ \text{inj} = \text{injection, at the nozzle} \]
\[ l = \text{liquid} \]
\[ n(\text{subscript}) = \text{nozzle} \]
\[ n(\text{superscript}) = \text{current time step} \]
\[ \text{rel} = \text{relative} \]
Chapter 4
Kinetic Chemistry Modelling

This chapter investigates the chemical reaction mechanism of Diesel fuel in a compression ignition engine with hydrogen-enriched air in order to identify and develop a chemical mechanism capable of accurately describing the co-combustion of hydrogen and Diesel and to identify whether or not direct chemical interaction between the overlapping coupled combustion reactions significantly impacts the overall combustion event.

4.1. Introduction

As shown in the preface, numerous investigations of the concurrent combustion of Diesel and hydrogen in compressions ignition engines have been conducted by various researchers. The majority of these investigations are of experimental nature, with only a limited number of computational models being available. While experimental engine test studies are of great benefit for verification of models and to determine the effect of specific parameter changes on the combustion, they only provide limited insight into the mechanisms affecting the co-combustion processes. Many of the available numerical studies, such as the studies by Shojae et al. [11] and Yang et al. [12], choose single-step global reactions for the Diesel and hydrogen combustion respectively without any proof of the validity of this approach.

Single-step global reactions do not allow for any communication between the combustion processes through their respective radical pool species, as these are not explicitly included in such models, which also limits the possible insights that may be gathered from these models. Further, when examining a detailed hydrocarbon combustion mechanism, such as
the 2885 species and 11,754 reaction Lawrence Livermore National Laboratory mechanism by Pei [79], it becomes easily apparent that the intermediate species of the hydrogen combustion, namely OH, H, H₂O₂, HO₂ etc., are involved throughout all stages of the Diesel reaction, from the initial reaction with the original fuel, reaction with the intermediate species, to the formation of the final reaction products. Elevated levels of these intermediate species occurring as a result of a concurrent hydrogen combustion may thus have significant influence on the Diesel combustion reactions. For example, Zhang et al. [80] found through a sensitivity study of a complex n-heptane mechanism that H₂O₂ greatly promotes the reaction rate, while HO₂ radicals are reaction inhibiting.

The motivation of this chapter is therefore to numerically study the effects hydrogen addition on the Diesel combustion to gain insight into whether chemical interaction of the hydrogen and Diesel mechanism radical and intermediate species is the foremost mechanism of interaction, or whether changes to the physical phenomena such flame speed, local equivalence ratios, local heat release, and fuel spray distributions are mainly responsible for these effects. This is achieved by comparing several combustion models of increasing complexity, as well as artificially decoupling the chemistry of the hydrogen combustion from the Diesel combustion, which is only possible computationally.

### 4.2. Computational Model Development

All computations were performed using a modified version of KIVA 3V release 2. All simulations presented here utilized the Renormalization Group (RNG) k-epsilon turbulence model [15] and the previously implemented Cascade Atomization and Drop Breakup (CAB) model [69], [50].
4.2.1. Engine Parameters and Inputs

The simulations presented in this study are based on the experimental work by Liew et. al. [9], [10], which were performed on a turbo-charged 1999 Cummins ISM 370 direct injected Diesel engine without exhaust gas recirculation (EGR). The following inputs were kept constant between the various simulations.

Table 4-1: Engine Specifications and Constant Inputs

<table>
<thead>
<tr>
<th>Engine</th>
<th>1999 Cummins ISM 370</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nr. of cylinders</td>
<td>In-line 6-cylinder</td>
</tr>
<tr>
<td>Displacement</td>
<td>10.8 L</td>
</tr>
<tr>
<td>Power rating</td>
<td>276 kW @ 2100 RPM</td>
</tr>
<tr>
<td>Bore</td>
<td>125 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>147 mm</td>
</tr>
<tr>
<td>Geometric Compression Ratio</td>
<td>16.5:1</td>
</tr>
<tr>
<td>RPM</td>
<td>1200</td>
</tr>
<tr>
<td>Load</td>
<td>70%</td>
</tr>
<tr>
<td>Initial Swirl</td>
<td>2880/min</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>218 mm</td>
</tr>
<tr>
<td>Initial Air Charge Temp. @ 40 deg bTDC</td>
<td>600 K</td>
</tr>
<tr>
<td>Piston Temp.</td>
<td>545 K (constant)</td>
</tr>
<tr>
<td>Cylinder wall Temp.</td>
<td>415 K (constant)</td>
</tr>
<tr>
<td>Cylinder Head Temp.</td>
<td>515 K (constant)</td>
</tr>
<tr>
<td>Injector arrangement</td>
<td>4 straight hole injector holes – angled 70° from vertical axis</td>
</tr>
<tr>
<td>Injector Hole Diameter</td>
<td>0.35 mm</td>
</tr>
<tr>
<td>Fuel Injection Temp.</td>
<td>330 K</td>
</tr>
</tbody>
</table>

Several simplifying assumptions were made for this study, whose limitations must be considered in evaluating the accuracy of the results. The wall temperatures were assumed to be constant throughout the cycle, affecting heat transfer. The initial flow field at 40 degrees bTDC was assumed to be purely rotational around the cylinder axis, neglecting any tumbling motion along the cylinder axis, which affects fuel distribution. The fuel injection event was
modelled as a square injection pulse, whereas real-world injectors mostly produce higher flowrates at the start of injection and trailing off as the injection pulse concludes. The use of the square pulse affects fuel concentrations, and thus reaction rates, especially at the beginning and end of the combustion event.

Between the 0% and 6% hydrogen case, all parameters were kept constant with the notable exceptions of the initial pressure at 40 degrees bTDC, the initial charge composition, and the start of injection crank angle. In the 6% hydrogen case, the initial pressure was reduced to match the experimental data, as the addition of hydrogen into the air intake stream reduces volumetric efficiency. The initial charge composition was altered to account for the added hydrogen. Finally, the start of injection was adjusted to account for the fact that the injection timing was allowed to shift according to the engine ECU in the experiment, as noted by the original researchers [10].

Additionally, it should be noted that in the experimental study, the Diesel fuel was reduced upon setting the desired hydrogen concentration, such that a constant load level, as defined by the measured engine power output, was achieved. The total fuel energy therefore differs notably between the 0% hydrogen case and the 6% hydrogen case, which has a reduced fuel input in terms of total energy.
Table 4-2: Varied Inputs

<table>
<thead>
<tr>
<th></th>
<th>0% vol H₂</th>
<th>6% vol H₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Pressure @ 40 deg bTDC</td>
<td>15.5 atm</td>
<td>14.6 atm</td>
</tr>
<tr>
<td>Mass of Diesel fuel</td>
<td>0.1425 g/cyl</td>
<td>0.0960 g/cyl</td>
</tr>
<tr>
<td>H₂ Mass fraction</td>
<td>0.00%</td>
<td>0.444%</td>
</tr>
<tr>
<td>H₂ Volume fraction</td>
<td>0.00%</td>
<td>6.00%</td>
</tr>
<tr>
<td>Start of Injection</td>
<td>5.5° bTDC</td>
<td>8.5° bTDC</td>
</tr>
<tr>
<td>End of Injection</td>
<td>21° aTDC</td>
<td>21° aTDC</td>
</tr>
</tbody>
</table>

4.2.2. Mesh and Mesh Independence

A structured 90-degree sector mesh with periodic boundaries was chosen due to the axial symmetry of the simulated cylinder and spray, in order to reduce computational cost of the simulation. The mesh is pictured in Figure 4-1.

Figure 4-1: Mesh with 45,642 cells at 40 deg. bTDC
Mesh dependence of the solution was investigated at mesh resolutions of 23,697 cells, 33,193 cells, 45,642 cells and 74,517 cells. Figure 4-2 depicts the average cylinder pressure using the same inputs for these mesh resolutions. It can be seen that the coarse meshes result in an over-prediction of cylinder pressure, which is likely due to smearing of the fuel concentration gradients near the jet. At a resolution of 45,642 cells, further mesh refinement did not result in any further changes to the solution and produced practically identical results and signifying mesh-independent of the solution. Synonymous results were observed for other parameters, such as average in-cylinder temperature, gaseous fuel concentrations, and other average species concentrations including, O, OH, H, CO\textsubscript{2} and H\textsubscript{2}O concentrations, which are not depicted here for brevity. Therefore, the 45,642 cell mesh was selected for all further simulations.

![Avg. Pressure vs Crank Angle](image)

**Figure 4-2: Avg. Pressure Mesh Independence Study**
4.2.3. Chemistry Solver

The kinetic chemistry solver inherent to KIVA was used for the global model reference simulations. This solver calculates the reaction rate based on the Arrhenius equation and then updates the species concentrations sequentially. The chemically reactions are thus only coupled by the concentrations at the beginning of each time step, which is sufficient for global and quasi-global reaction mechanisms but can present issues for larger detailed mechanisms with hundreds of reactions.

One such issue is the failure to initiate the reaction if initial species concentrations are zero, as the mathematical scheme fails to move on from the null solution, thus requiring an arbitrary small initial value for the solution to proceed. Intermediate species, especially if short-lived, only ever exist in small concentrations, meaning small arbitrary initial inputs may alter the solution.

Further, the KIVA solver does not consider backwards reactions, unless explicitly specified. In contrast, CHEMKIN will calculate backwards reactions from the equilibrium constants derived from thermodynamic data [16]. As the CHEMKIN format is practically the standard today for complex mechanisms publications, the same thermodynamic data and backwards-reaction calculations would have to be implemented in KIVA to achieve comparable results between the two solvers to utilize complex mechanisms.

On the other hand, simple global mechanisms do not predict ignition delays accurately. Empirical ignition delay models, such as Correa’s approach of correlating CO concentrations to model ignition delay, as CO stays essentially zero during ignition delay period and rises
sharply at the ignition event [25], are often used to remedy this short-coming, but are not implemented in the standard KIVA code-set.

Finally, detailed reaction mechanisms commonly include three-body reactions and pressure-dependent reactions, such as unimolecular/recombination fall-off reactions. These mechanisms are not natively available in the original KIVA code set and were thus implemented.

For three-body reactions, the concentrations of such non-reactive third body species are simply added to the rate expressions akin to the reactive species, multiplied by an efficiency factor to account for different interaction efficiencies of the various species [16].

For pressure-dependent unimolecular / recombination fall-off reactions flowing the Lindemann approach [81], it is required to specify Arrhenius rate expression for both the low pressure limit, \( k_0 \), and high pressure limit, \( k_\infty \).

\[
k_0 = A_0 T^{\beta_0} \exp\left(-\frac{E_0}{R_u T}\right) \quad (4.1)
\]

\[
k_\infty = A_\infty T^{\beta_\infty} \exp\left(-\frac{E_\infty}{R_u T}\right) \quad (4.2)
\]

Where \( A \) is the pre-exponential factor, \( T \) is the temperature in Kelvin, \( \beta \) describes non-linearity in temperature dependence, \( E \) is the activation energy, and \( R_u \) is the universal gas constant.
The reaction rate constant at any pressure is then expressed based on the reduced pressure

\[ P_r = \frac{k_0[M]}{k_\infty} \]  

(4.3)

as

\[ k = k_\infty \left( \frac{P_r}{1+P_r} \right) F \]  

(4.4)

In rate expressions conforming to the Lindemann form, the shape factor \( F \) is unity. If \( F \) is not unity, the expression is in non-Lindemann form and is determined by the Troe fall-off function as follows [82].

\[ \log F = \left[ 1 + \left( \frac{\log P_r + c}{n - d \log (P_r + c)} \right)^2 \right]^{-1} \log F_c \]  

(4.5)

where

\[ c = -0.4 - 0.67 \log F_c \]  

(4.6)

\[ n = 0.75 - 1.27 \log F_c \]  

(4.7)

\[ d = 0.14 \]  

(4.8)

\[ F_c = (1 - \alpha) \exp \left( -\frac{T}{T^{**}} \right) + \alpha \exp \left( -\frac{T}{T^*} \right) + \exp \left( -\frac{T^{**}}{T} \right) \]  

(4.9)

Here, the values of \( \alpha, T^{***}, T^* \), and \( T^{**} \) are empirically determined user-defined inputs.
The simulations presented in this paper utilizing the larger reduced kinetic mechanisms containing more than 100 individual reactions were performed by fully integrating the CHEMKIN code set [16], [83] into KIVA, following the work by Ra and Reitz [84]. CHEMKIN sets up and solves the fully coupled Ordinary Differential Equations (ODEs) resulting from the kinetic mechanism.

The code is set up to directly read in CHEMKIN mechanism files and solve the constant volume combustion for each computational cell at each time step. The integration of CHEMKIN provides improvements in stability and accuracy of the results over the standard KIVA chemistry solver, however, the higher computational requirements of repeatedly solving large numbers of coupled ODEs comes at a significant computational cost, especially as the kinetic mechanism become more refined and extensive.
4.3. Chemical Kinetic Model

4.3.1. Fuel Models

Diesel fuel consists of hundreds of individual constituent species, including mainly saturated hydrocarbons (~75%) and to a lesser degree aromatic hydrocarbons (~25%), averaging in length around the C12 level [85]. The exact composition may vary greatly between various Diesel fuel products, summer vs. winter formulations, and geographic regions.

Especially less complex combustion models, such as global and reduced reaction mechanisms, therefore require the definition of a single reference fuel with similar characteristics to the actual Diesel fuel mixture. Diesel is therefore commonly modelled as the dodecane (C\textsubscript{12}H\textsubscript{26}) based DF2 model [86] used in KIVA, which matches the average molecular weight of Diesel, or as n-heptane (C\textsubscript{7}H\textsubscript{16}) [84], [87], which matches the heating value and combustion characteristics of Diesel fuel very well, despite its lower molecular weight.

A common practice for such fuel models is to separate the physical and chemical properties of the fuel, such that the chemical properties of the chemical species are retained to calculate the chemistry, but utilize empirical data of the physical properties, such as density and surface tension, from the actual Diesel fuel to compute physical processes of the fuel injection and break-up processes. This approach is used both by the KIVA DF2 model, as well as the n-heptane model described in this paper.
With the development of increasingly complex detailed reaction mechanisms, many now spanning tens of thousands of reactions and thousands of species, multi-component fuel models are being investigated [79], [88], but require highly detailed reaction mechanisms.

### 4.3.2. Reaction Mechanism

Chemical reaction mechanisms can be roughly grouped in three categories: global, skeletal/reduced, and detailed mechanisms.

Global mechanisms are the most simplistic, consisting of a single irreversible kinetic reaction step for the conversion of fuel to products. Similarly, quasi-global models expand these global models to a limited number (~5) of reaction steps. While computationally inexpensive, these mechanisms provide no details on the evolution of intermediate species, nor can the reaction time be determined, as the reactants are converted to products instantaneously in the same step. Since intermediate species are not considered in global mechanisms, no chemical interaction is possible between two concurrently reacting fuels.

On the other end of the spectrum are detailed mechanisms. For complex hydrocarbon combustions, these may include up to tens of thousands of reactions and thousands of intermediate species. Such detailed mechanisms include the 990 species, 4060 reaction mechanisms by Curran et. al. [89], which is based on the combination of a H\textsubscript{2}/O\textsubscript{2} mechanism with a C1-C8 mechanism, but not including aromatic hydrocarbons, to model a surrogate fuel comprised of n-heptane and iso-octane; and the Lawrence Livermore National Laboratory mechanism by Pei, which includes 11754 reactions and 2885 species [79].
For a detailed hydrogen mechanism, such as the San Diego Mechanism developed by Saxena [90], the mechanism is significantly less complex due to the lower complexity of the fuel and much lower number of intermediate species, containing only eight species and 21 reactions.

Due to their computational expense, these mechanisms are primarily utilized for 0-D combustion calculations and Direct Numerical Simulations (DNS) of simple geometries. As noted by Nordin, detailed chemistry requires detailed physical models [91], as otherwise the computational expense does not justify the additional accuracy of the chemical models outweighed by the accuracy limitations of the physical models, and are therefore rarely used for complex engine simulations. However, Nordin used probability density functions coupled with Large Eddy Simulations (LES) to model interaction between turbulence and chemistry [24] in order to simulate reasonably detailed chemical models and alleviate the limitations of the more traditional RANS simulations.

Skeletal and reduced models aim to find a compromise between computational expense and accuracy, while retaining the major intermediate species. These mechanisms are obtained by combining, grouping, and/or deleting reactions from detailed mechanisms based on various sensitivity analysis methodologies. This, however, may make the mechanism only suitable for certain pressure, temperature or operating ranges, e.g. either low or high temperature ignition, reducing the general applicability of mechanism. The range of complexity of these reduced mechanisms is quite broad. For example, Frassoldati et. al. reduced a multi-component surrogate fuel mechanism of initially 451 species and 17,747 reactions to 123
species and 1017 reactions [88], while the reduced n-heptane/toluene mechanism developed by Chen et al. contains only 60 species and 145 reactions [92].

4.3.3. Model Description

The Arrhenius rate coefficient, \( k(T) \), is determined by the pre-exponential factor \( A \), the temperature exponent \( b \), and the activation energy \( E_a \), which in the KIVA input format already includes division by the gas constant.

For models M1, M2 and M3, with the pre-divided the activation energy value, \( E_a \), and using KIVA input units, the Arrhenius equation becomes:

\[
k(T) = A T^b \exp\left(\frac{-E_a}{T}\right)
\]  

(10)

On the other hand, models M4 and M5, which utilize the CHEMKIN solver, list the activation energy prior to division by the universal gas constant, as required by the CHEMKIN input format, such that the following equation applies.

\[
k(T) = A T^b \exp\left(\frac{-E}{R_uT}\right)
\]  

(11)

Accordingly, the units for models M4 and M5, as listed in Table A-2 and Table A-3, are mole-cm-sec-K for the pre-exponential factor, \( A \), and cal/mol for the activation energy, \( E \).
4.3.4. Model M1

The first model investigated is the standard KIVA DF2 model, as commonly used for Diesel engine simulations. This model consists of a single irreversible global Diesel reaction,

$$2 \text{C}_{12}\text{H}_{26} + 37 \text{O}_2 \rightarrow 24 \text{CO}_2 + 26 \text{H}_2\text{O} \quad (\text{M1.1})$$

where the Arrhenius coefficients are $A = 3.0\text{E}+11$, $E_a = 1.7614\text{E}+4$, $b = 0.0$ in KIVA input units of mole, cm, s.

Further, four reversible equilibrium reactions for hydrogen are applied, which are usually used to describe the emission gas composition. The standard Kiva solver was utilized for this model.

$$\text{H}_2 \leftrightarrow 2 \text{H} \quad (\text{M1.2})$$

$$\text{O}_2 \leftrightarrow 2 \text{O} \quad (\text{M1.3})$$

$$\text{O}_2 + \text{H}_2 \leftrightarrow 2 \text{OH} \quad (\text{M1.4})$$

$$\text{O}_2 + 2 \text{H}_2\text{O} \leftrightarrow 4 \text{OH} \quad (\text{M1.5})$$

Since the Diesel reaction omits any intermediate species, there is no interaction direct chemical between the Diesel and hydrogen mechanism in this model.
4.3.5. Model M2

The same global kinetic Diesel model and chemistry solver are used as in Model M1, such that again no chemical interaction between the Diesel and hydrogen reactions exists. The hydrogen equilibrium reactions M1.2 through M1.5 are replaced by a single irreversible global hydrogen reaction based on the work by Marinov [93].

\[
2 \, H_2 + O_2 \rightarrow H_2O
\]  \hspace{1cm} \text{(M2.1)}

where the Arrhenius coefficients are \( A = 1.8E+13 \), \( E_a = 1.5078E+4 \), \( b = 0.0 \) in KIVA input units of mole, cm, s.

4.3.6. Model M3

For model M3, the single-step KIVA DF2 model is combined with a fairly detailed, reduced hydrogen mechanism developed by Boivin [94], consisting of twelve reactions, six of which are reversible with the backwards reactions explicitly defined, as described in Table A-1. The KIVA solver was utilized for these simulations, though the occurrence of third-body interactions and Troe-centered pressure dependence of the reaction required the use of the extensions to the KIVA solver discussed previously. Due to the global Diesel mechanism without intermediate species, again no chemical interaction between the Diesel and hydrogen mechanism exists.
4.3.7. Model M4

Model M4 utilizes a reduced n-heptane Mechanism consisting of 35 species and 119 reversible elementary reactions and utilizes the fully integrated CHEMKIN solver. The model is based on the work by Ra et al. [84] and is described in Table A-2. The only modification to the model was the removal of the unused iso-octane reaction branch and the enhancement of the CO reaction rate in reactions M4.26-M4.29, as CO oxidation was found to otherwise not significantly occur. This is a valid methodology, as the reaction rate coefficients not only can vary significantly depending on the experimental or computational methodology by which they are determined, but can also be mesh dependent, as pointed out by Amsden [86].

Since the detailed model includes a hydrogen mechanism, described by reactions M4.108 through M4.119, as part of the Diesel mechanism, a separate hydrogen model is not required, yet providing full communication between the hydrogen and Diesel chemistry. However, the tracking of the additional intermediate species and significantly more complex chemistry comes at a considerable computational cost, increasing computational times by about a factor of ten when compared to models M1 through M3.

Finally, in a separate simulation, the hydrogen mechanism was decoupled from the reaction mechanism by creating duplicate dummy species and reactions of all hydrogen reactions and intermediate species with the same thermodynamic properties and reaction coefficients. This allowed for the investigation of the hydrogen reaction to occur using the same parameters but remaining mathematically separated from the Diesel radical pool. This decoupling added seven species and twelve reactions to the mechanism.
4.3.8. Model M5

Since the hydrogen mechanism in model M4 was only intended for the reaction of the intermediate species, which only ever occur in small quantities compared to the case of hydrogen enrichment, it was necessary to verify the applicability of the model to higher hydrogen concentration ranges, particularly for the decoupled case. Therefore, the hydrogen mechanism, M4.108 – M4.119, was replaced by a more complete mechanism developed by Saxena [90] and specified by reactions M5.108 – M5.128 in Table A-3, which was specifically designed for the combustion of hydrogen in air.

A chemically decoupled simulation of this mechanism was investigated as well, which resulted in the further addition of eight species and 21 reactions to the model.

4.4. Discussion of Results

The average in-cylinder pressure evolution for model M1, which uses a global Diesel kinetic reaction and hydrogen equilibrium reactions, is depicted in Figure 4-3 for both the 0% and 6% hydrogen case and compared to the experimental results as published by Liew et al. [9]. A significant over-prediction of the maximum pressure can be observed in both cases, along with an early rise in pressure. This signifies that combustion is predicted by this model to start too early, at about 5 degrees before Top Dead Center (bTDC), as no ignition delay model is employed. However, the relative increase in maximum pressure between the 6% hydrogen case and the 0% hydrogen base case is fairly well matched.
Similarly, Figure 4-4 depicts the pressure profile for the kinetic hydrogen models performed in KIVA, M2 and M3. Since the Diesel model is the same as in M1, the 0% hydrogen case shows the same behavior of early ignition as observed in M1. The single irreversible hydrogen reaction in M2, however, predicts a nearly instantaneous reaction of the hydrogen and consequent pressure rise at 10 degrees bTDC, as a result of the irreversibility of the reaction and the fact that ignition delay and reaction duration of elementary reactions are not modelled. With the extension of the hydrogen mechanism in model M3, it is observed that the pressure increase is closely tied to that of the pure Diesel reaction. This suggests that the hydrogen does not auto-ignite, but only reacts due to the energy of Diesel heat release. While the maximum pressure for M3 matches the experimental data within 1.65% and occurs
within 4 degrees crank angle of the experimental maximum pressure, this is mostly coincidental due to the early ignition of the Diesel.

![Graph showing Avg. Pressure vs Crank Angle](image)

**Figure 4-4: Model M2 and M3, KIVA kinetic hydrogen mechanisms**

Model M4, containing the detailed chemistry for both the hydrogen and the Diesel mechanism, as depicted in Figure 4-6, shows a vast improvement over the previous models, especially with respect to the early Diesel ignition. The 0% hydrogen case matches the maximum pressure within 0.56% and its occurrence within 1.5 degrees crank angle of the experimental data. The 6% hydrogen case matches the maximum pressure within 1.73% and its occurrence within less than 0.5 degrees crank angle of the experimental data. In both cases the start of the pressure rise is well predicted, although in the 6% hydrogen case, the rate of pressure rise lags somewhat within the first five degrees aTDC, while pressure is slightly overestimated for 0% hydrogen case between 20 and 30 degrees aTDC. These minute
differences are easily explained by the simplifying assumptions, especially the initial flow field and the square injection profile used for these simulations.

The decoupled chemistry model clearly shows a failure to ignite the mixture represented by the only minor pressure increase from chemical heat release. The Diesel fuel charge being significantly reduced leads to exceedingly lean conditions, and the hydrogen is unable to auto-ignite without access to the radical pool of the Diesel combustion nor the heat release from the Diesel reaction due to the Diesel ignition failure. These results therefore strongly indicate that direct chemical interaction between the Diesel and hydrogen combustion occurs and should be accounted for when modelling compression ignition dual fuel engines.

Figure 4-7 depicts the in-cylinder temperature distributions for model M4 for both the 0% and 6% hydrogen cases and their evolution over time. At Top Dead Center (TDC, 0° crank angle), a drop in temperature at the center of the Diesel spray jet due to evaporation is observable. The region of elevated temperatures between the cylinder wall and piston head signifies the early stages of fuel ignition occurring at this time. A slight delay in ignition timing is observable in the 6% hydrogen case, which is in agreement with the pressure plots in Figure 4-5.

As the ignition proceeds to sweep the cylinder between 5° and 15° CA (crank angle), the hydrogen enriched case shows significantly elevated temperatures compared to the pure Diesel case. At 30° CA, the highest temperatures in the pure Diesel case remain mostly confined to the outside of the cylinder, while in the hydrogen-enriched case, the high temperature region has migrated further towards the center of the cylinder.
The extended hydrogen model in model M5, depicted in Figure 4-6, shows nearly identical results to M4. For the 0% hydrogen case, the predicted maximum pressure is within 1.4% of the experimental data, however, it is predicted to occur about 3 degrees early. The crank angle maximum pressure in the 6% hydrogen case is well matched, and has a value within 2.48% of the experimental data.
While the decoupled simulation for this model shows a somewhat higher pressure rise and thus chemical heat release than model M4, full combustion is not achieved in this case either. This further supports the findings that chemical interaction of the intermediate species and radical pool is of significant importance, as well as justifying the use of the reduced hydrogen model in M4 for simulations with elevated hydrogen levels.

**Figure 4-6: Model M5 coupled and decoupled**
Figure 4-7: Temperature distribution, Models M4
4.5. Chemical Interactions

The local high variability of conditions in space and time, including local species distributions, locally varying temperatures and pressures, and flow movements in a complex geometry process such as a moving piston engine simulation makes a direct detailed investigation of the chemical reactions impossible.

Therefore, the previously discussed model M4 was simulated for a control volume of simple geometry directly using CHEMKIN without the use of KIVA. The simulation constituted a constant volume, well-stirred combustion with adiabatic wall conditions using air as the oxidizer and a stoichiometric mixture of equal amounts by volume of gaseous Diesel (n-Heptane) and hydrogen. The initial conditions were chosen to roughly represent the top dead center conditions of the Cummins ISM 370 engine prior to ignition, such that the initial temperature was 1000 K and the initial pressure was 8000 kPa. The simulation was carried out for both the coupled chemistry case and the decoupled chemistry case. For the decoupled case, hydrogen and its intermediate species were modeled using dummy species not occurring in the Diesel mechanism. These dummy species were assigned the same properties as the original species and only serve to separate the Diesel combustion species form the hydrogen combustion species.

The results for the coupled case are shown in Figure 4-8, with Figure 4-9 providing a zoomed in version at the time of the main reaction event. Figure 4-10 shows the same results for the decoupled chemistry case. For this figure it should be noted, that species described in the legend represent those of the standard Diesel combustion mechanism, while the “Total” species include the contributions from both the Diesel and the hydrogen reaction.
The chemical reaction process of hydrocarbons can, at its most basic, be subdivided into three phases. The chain initiating reactions start the reaction by breaking down the reactants into radicals and smaller hydrocarbons and include the process of H-abstraction. The initiating reactions are generally endothermic, as energy is required to initially break the existing bonds. This is followed by chain branching and/or chain propagating reactions that further the reaction. Finally, the chain terminating or recombination reactions result in the formation of the final products and mark the phase of greatest heat release.

For the coupled reactions in Figure 4-8, the reactions progress slowly between 0 and 1.0E-4 seconds. This phase is dominated by the chain initiating reactions. Between 1.0E-4 to 1.2E-4 seconds, the reactions rapidly progress, resulting in a large temperature increase and the formation of the final products. After 1.2 E-4 seconds, the species remain in equilibrium.
Figure 4-9 presents the a more detailed view of the species during the main combustion event around 1.4E-4 seconds. Since the initial mixture is stoichiometric, oxygen rapidly decreases, while the products H$_2$O and CO$_2$ increase equally rapidly, along with temperature. HO$_2$ remains at very low levels throughout the reaction, while OH only appears with the formation of the products, as it is consumed by the reactions prior to this point. Just prior to the point of maximum reaction rate, hydrogen increases above the initial levels due to the liberation of hydrogen atoms from the hydrocarbon fuel. At the same time, H$_2$O$_2$, is depleted just prior the point of maximum heat release rate.
The reaction for the chemically decoupled case looks very different. The first notable difference is the significantly longer reaction time. The main Diesel reaction occurs between 2.4E-4 and 4.4E-4 seconds and the heat release rate is significantly reduced compared to the coupled case. At around 4.4E-4 seconds, a nearly instantaneous reaction occurs for the decoupled hydrogen. Overall, the temperature remains lower than in the coupled case. While the species concentrations for most of the species evolve qualitatively similar to the coupled case, albeit at a longer time scale and with a step jump at the occurrence of the hydrogen
reaction, H$_2$O$_2$ behaves markedly different. While in the coupled case, H$_2$O$_2$ remains fairly constant after its initial production up to the point of maximum heat release rate, in the decoupled case H$_2$O$_2$ continuously builds up until about 3E-4 seconds, then declines somewhat as the Diesel reactions accelerate, but significant amounts remain even after the hydrogen step reaction occurs. Since the H$_2$O$_2$ and Total H$_2$O$_2$ plots exactly overlay, it is apparent that the H$_2$O$_2$ is entirely a byproduct of the Diesel reaction.

Figure 4-10: Kinetics Study M4 Decoupled
This analysis of the, albeit relatively simplistic reaction mechanism compared to other detailed Diesel combustion mechanisms, therefore suggests that there are significant chemical interactions between the concurrent oxidation reactions of Diesel and hydrogen and further suggests that one of the major mechanisms of this interaction is through H$_2$O$_2$.

As noted previously, Zhang et al. [80] found through a sensitivity study of a complex n-heptane mechanism that H$_2$O$_2$ greatly promotes the reactions of n-heptane. Based on this finding and the results presented above, the proposed interaction mechanism is as follows.

a) The Diesel reactions produce an excess of H$_2$O$_2$.

b) The excess H$_2$O$_2$ supplements the radical pool of the hydrogen reactions.

c) The short mechanism with relatively few sub-steps and short reaction times provides a “shortcut”, i.e. an alternative reaction route with short reaction times, for the production of the final product H$_2$O.

d) The production of H$_2$O results in increased heat release in the early stages of the reaction.

e) The additional heat from the production of H$_2$O through the oxidation of the additional hydrogen provides the necessary energy to raise the temperature of the gas mixture and increase the Diesel reaction rates, thus accelerating both reactions.

In the previous section, it was observed that the decoupled mechanism did not result in a full combustion event. This may be explained by the diffusion of heat into the surrounding volume, preventing the hydrogen reaction from being initiated.
4.6. Conclusions

Several combustion models for the Diesel/hydrogen co-combustion, along with different chemistry solvers were computationally tested and compared under the same conditions for a 0% and a 6% hydrogen enhancement case and compared to literature data.

A single-step global kinetic Diesel reaction, paired with four hydrogen equilibrium reactions using the standard KIVA chemistry solver, was able to fairly accurately predict the relative pressure rise resulting from the hydrogen enhancement, but the Diesel mechanism failed to predict the ignition timing, resulting in overall overprediction of the in-cylinder pressures.

The single-step global kinetic Diesel reaction paired with a single-step global kinetic hydrogen reaction using the standard KIVA solver, not only failed to predict the ignition timing, but erroneously predicted a nearly instantaneous and complete reaction of the hydrogen.

A single-step global kinetic Diesel reaction paired with a 12-step kinetic hydrogen model utilizing a modified and extended version of the KIVA solver was able to predict the maximum pressure for the hydrogen-enhanced case within 1.65%, but the hydrogen reaction was only perpetuated as a result of the Diesel reaction, rather than being self-propagating after the point of ignition. The failure to predict ignition timing of the Diesel mechanism persisted, resulting in overprediction of the maximum pressure in the pure Diesel case.

A detailed, reduced n-heptane mechanism consisting of 119 reversible kinetic reactions including an 11-step hydrogen mechanism and utilizing the fully integrated CHEMKIN chemistry solver was able to predict ignition delay, maximum in-cylinder pressure within
1.73% and crank angle of maximum pressure within 0.5 degrees crank angle. The validity of the use of the hydrogen mechanism at elevated hydrogen concentrations was confirmed by replacing the 11-step hydrogen mechanism with a 21-step mechanism specifically developed for hydrogen combustion, which showed only minor differences. However, the use of the detailed mechanisms and CHEMKIN integration came at a significant computational cost increase.

Decoupling of the hydrogen and Diesel chemistry resulted in failure to ignite and combust the mixture. The results therefore strongly suggest that there is significant direct chemical interaction between the Diesel and hydrogen radical pools and intermediate species and must be accounted for, such that chemistry models for Diesel/hydrogen co-combustion simulations without communication between these reactions should only be used with great caution.

The addition of 6% hydrogen caused a slight delay in the ignition of the mixture, despite advancement of the injection timing. The maximum pressure under these operating conditions was increased by about 15% compared to the maximum pressure of the pure Diesel case, due to significantly increased combustion temperatures. A shift of the high temperature combustion zone away from the cylinder wall and towards the cylinder center was also observed with the addition of hydrogen.

A detailed investigation of the coupled and decoupled Diesel and hydrogen reactions in a constant volume process suggest that the concurrent oxidation reactions are significantly coupled through the exchange of H$_2$O$_2$ between the two radical pools.
Chapter 5  
Parametric Study of Hydrogen Direct Injection Strategies

This chapter presents a parametric study to compare the performance of a dual fuel compression ignition engine with a Diesel main fuel and hydrogen pilot fuel for select cases of hydrogen ingestion into the intake air with various direct hydrogen injection strategies. The computational results are compared for their thermodynamic cycle performance to determine efficiency. This analysis aims to determine how hydrogen enrichment effects the thermodynamic cycle performance, and whether or not direct hydrogen injection produces a net benefit on fuel efficiency compared to hydrogen intake ingestion and at which point these strategies become theoretically feasible. A full optimization of the system, the physical design of the injector, and comprehensive emission mitigation studies fall outside of the scope of this investigation.

5.1. Introduction

Direct fuel injection systems have displaced carbureted engines for nearly all modern automotive applications, owing to the superior fuel efficiency and emissions of the stratified charge combustion. Operating on the same basic principle, it is easy to draw the analogy of carbureted engines to hydrogen ingestion into the intake air. The next logical step in the investigation of hydrogen pilot fuels is thus the switch from ingested to direct injected hydrogen.
The direct injection of hydrogen as a pilot fuel in Diesel engines has not been widely studied at this time and literature on this topic is sparse. For example, Gürbüz investigated various hydrogen direct injection strategies, including multiple injection pulses, by utilizing a 1-D direct hydrogen injection model [95]. The results of this study showed that engine power was significantly increased, while simultaneously reducing soot emissions, but at the expense of slightly elevated NOx emissions. Kavtaradze [96] performed numerical 3-D simulations on a hydrogen Diesel engine with direct hydrogen injection and similarly found that the engine produced an indicated efficiency of 48% at a hydrogen supply rate of 0.49 g/cycle, but the production of NOx presented a challenge.

5.2. Concept

Based on the laws of thermodynamics, every transformation of energy from one state to another, e.g. converting thermal energy to mechanical energy or electrical energy, is always associated with losses in a closed system. It therefore appears counterintuitive to extract useful work from an engine, only to turn it back into fuel for that same engine, as the losses in each conversion step would quickly reduce the recycled fuel energy available.

However, the manner in which energy in the form of chemical fuel is added in an internal combustion engine has major implications on its overall thermodynamic cycle performance. In the previous chapter, it was shown that hydrogen enrichment increases ignition delay and increases the speed of the chemical kinetic reactions of the combustion process. This chapter investigates how these two effects of hydrogen enrichment modify the thermodynamic cycle of the engine. The possible scenarios that would lead to an increase in engine efficiency are as follows.
Diesel engines require fuel injection during the compression stroke, such that the fuel has time to evaporate and produce a combustible gaseous fuel-air mixture that allows for auto-ignition. As depicted in the simplified sketch of rate of heat release (ROHR) vs crank angle in Figure 5-1, if the fuel is injected early, heat release and consequently pressure rise may occur due to premixed combustion prior to top dead center of the piston, which not only reduces the work produced in the expansion stroke, but also creates additional negative work during the compression stroke. Especially in older, low injection pressure engines with early fuel injection, this may lead to notable losses, that are unavoidable due to the time requirements of the fuel vaporization to make ignition possible. In that case, the ignition delay caused by the hydrogen enrichment would push the premised ignition phase further into the expansion stoke, while allowing more time for fuel vaporization. However, the experimental results by Liew et al. [9] show that cylinder pressure does not rise above the motoring pressure until after TDC, meaning that for the Cummins ISM 370 engine in these studies, the effect of early ignition is not a factor, as the engine uses high injection pressures and relatively late injection timing leading to a well-timed ignition crank angle.
Another theory often suggested in literature on hydrogen enrichment is that the hydrogen improves combustion efficiency. As pointed out by Heywood [97], Diesel engines always operate lean and thus generally have a combustion efficiency of roughly 98%. In fact, Liew et al. found experimentally that the combustion efficiency of the Cummins ISM 370 engine at 1200 rpm and 70% load was upwards of 99.5% and marginally deteriorated with increasing hydrogen enrichment. Improvements in combustion efficiency therefore cannot explain the relatively large efficiency improvements through hydrogen enrichment reported in literature.

Figure 5-1: Sketch of Rate of Heat Release for combustion phases
This leads to the thermodynamic cycle efficiency. The theoretical ideal Otto cycle is inherently more efficient than the ideal Diesel cycle when compared at the same compression ratio, as depicted in Figure 5-2. For practical applications, however, the Diesel cycle allows for significantly higher compression ratios, making the Diesel cycle more efficient than the Otto cycle in real world applications. The ideal engine would therefore operate on the Otto cycle, but under Diesel compression ratios, which is already fairly closely approximated by real world Pressure-Volume (P-V) diagrams of practical Diesel engines. By increasing the ratio of premixed combustion to mixing-controlled combustion, the real world Diesel engine cycle approaches the Otto cycle.

Figure 5-2: Comparison of air-standard Otto cycle, Dual cycle, and Diesel cycle with same input conditions and same compression ratio [98]
Conventional Diesel engines already utilize pilot injection strategies. The goal of these pilot fuels is to create pre-mixed charge that is already evaporated and burns quickly at the point of the main fuel ignition, thus creating the necessary heat to evaporate and ignite the main fuel charge and ultimately increase the heat release in the premixed combustion phase. The same principle is sought with direct hydrogen injection pilot fuels, although since Diesel auto-ignites more easily than hydrogen, the Diesel first has to act as the ignition source for the hydrogen pilot. Hydrogen enrichment, either through ingestion into the intake air, or through early pilot direct injection, therefore more closely approximates the Otto cycle constant volume heat addition through three mechanisms:

1) A larger fraction of the fuel is introduced early and in gaseous form, making it immediately available at the time of ignition and during the premixed combustion phase, effectively being equivalent to an advancement in fuel injection timing.

2) The hydrogen enrichment causes an increased ignition delay, which allows for earlier Diesel injection, such that more Diesel fuel can evaporate and combust in the premixed combustion phase.

3) Intermediate species of the hydrogen and Diesel combustion chemically interact to cause an increase in kinetic reaction rates and thus increased heat release rates.

These three effects occur simultaneously, leading to faster combustion rates and therefore a closer approximation of the constant volume heat addition process of the Otto cycle, compared to conventional real-world Diesel operation.
5.3. **Numerical Model**

The computational study presented in this chapter is based on the combined models presented in the previous chapters and utilizes the same Cummins ISM 370 engine geometry, parameters and computational mesh described in Figure 4-1 and Table 4-1. For comparability of the results, the Diesel injection timing is held constant for all cases presented here. As hydrogen is known to delay the ignition timing, the advanced Diesel injection timing of the 6% hydrogen case in the previous chapter with a start of injection (SOI) of -8.5°CA to end of injection (EOI) of + 21°CA was chosen. Similarly, the initial pressure at 40° bTDC was held at 14.6 atm for all cases, as in the 6% hydrogen case in the previous chapter.

Hydrogen is injected via a square injection pulse. For all simulations, it is assumed that injection pressure remains exactly at the critical pressure ratio, such that the injector remains choked throughout the injection event to calculate injection velocity based on the compressible 1D model presented in Chapter 2. The critical pressure assumption was made for this analysis in order to minimize the energy necessary to compress the hydrogen while maintaining choked flow.

The only parameters adjusted in this study are therefore the respective mass of the Diesel and hydrogen fuels and the hydrogen injection timing, i.e. the start and end crank angle of the hydrogen injection event, as well as the method of introducing the hydrogen into the cylinder, which are described in Table 5-1. For simplicity, column a) in this table refers to either the volume fraction of hydrogen at the start of the simulation for the hydrogen ingestions cases, or alternatively to the equivalent hydrogen mass for the direct hydrogen
injection cases. The fuel mass per cylinder per power stroke for Diesel and hydrogen are given in columns e) and f) of Table 5-1.

It is of great importance to emphasize at this point, that the total energy input as chemical energy through the Diesel and hydrogen fuels is NOT constant between cases of different hydrogen enrichment levels. In the experimental study by Liew et al., the desired hydrogen concentration in the intake air was set, upon which the Diesel fuel was reduced until the load condition in terms of power output as measured by a dynamometer was achieved [9]. For consistency of these literature results with the work performed in this dissertation, the same variable Diesel and hydrogen amounts were used for this study as described by the literature [12].

In Table 5-1, case A.0 demarks a reference case with the advanced injection timing, but without any hydrogen addition to the system. Cases A.1 through A.4 investigate the effects of hydrogen addition through ingestion into the intake air at various hydrogen levels, while maintaining constant Diesel injection timing. Cases B.1 through B.4 feature various levels of hydrogen direct injection through a dual cone injector, where the inner solid cone with an initial cone angle of 15° consists of hydrogen, and Diesel is injected as an outer hollow cone with an initial total spray angle of 35°, as depicted in Figure 5-3. In these cases, the hydrogen and Diesel injection timings are identical, meaning that hydrogen is injected throughout the Diesel injection event.
Similarly, cases C.1 through C.4 study the effects of various hydrogen levels at constant hydrogen injection timing for a mixed cone with initial cone angle of 30°, i.e. the Diesel and hydrogen are assumed to be concurrently injected through the same nozzle akin to an air-blast atomizer design. The remaining cases C.4 through C.11 investigate the effects of varying hydrogen injection timing utilizing the same mixed cone setup.

Figure 5-3: Dual cone definition
### Table 5-1: Hydrogen Injection Parameters

<table>
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<th>Case</th>
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<th>H2 inj. nozzle</th>
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<th>EOI H2 deg. CA</th>
<th>Mass (Diesel) [mg/cyl]</th>
<th>Mass (H2) [mg/cyl]</th>
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</table>
5.4. Results

The results of the parametric study are summarized in Table 5-2. Column a) lists the indicated engine power per cylinder at 1200 rpm, which is depicted in Figure 5-5 and was calculated by integration of the PV diagram for each case by assuming closed valves throughout the full (360 degree) engine revolution and no friction losses or pumping losses, as illustrated by Figure 5-4.

![Sample PV Diagram](image)

**Figure 5-4: Sample PV Diagram**

Column b) lists the percent change in engine power relative to the reference case A.0, in which the Diesel injection timing is consistent with the remaining cases, but no hydrogen enhancement is present.
Columns c) and d) list the fuel energy per cylinder per power stroke of the Diesel and hydrogen fuel respectively, based on the fuel masses provided in Table 5-1 and a lower heating value of 44,926 kJ/kg for n-heptane [99] and 120,000 kJ/kg for hydrogen [98]. Column e) describes the sum of the hydrogen and Diesel rate of fuel energy per cylinder in kJ/s for the given operating condition of 1200 rpm.

Column f) calculates the indicated efficiency, depicted in Figure 5-6, based on the engine power (a) and total fuel energy (e). This efficiency is representative of the case where hydrogen is supplied by a secondary fuel tank, or alternatively, if the hydrogen is produced by recovered energy from regenerative braking, waste heat, or other sources.

\[
\eta_{\text{indicated}}\% = \frac{\text{Engine Power}}{\text{Total Fuel Energy}} \times 100\% \quad (5.1)
\]

The efficiency listed in column g) on the other hand is calculated under the assumption that mechanical power from the engine is used to generate and compress the hydrogen, where the hydrogen generation and compression are ideal processes. In particular, it is assumed that there are no energy conversion losses in converting the mechanical engine power to electrical power, the energy rate for hydrogen generation through, for example electrolysis, is 100% efficient and is given by \( \dot{E}_{H_2} \), and work required for the hydrogen compression, \( W_{\text{comp}} \), is for simplicity roughly estimated by isentropic compression based on the maximum in-cylinder pressure during the hydrogen injection event listed in column h). For hydrogen ingested into the intake air, the hydrogen does not need to be pre-compressed, such that compressive work for this case is zero.

\[
\eta_{\text{ideal}}\% = \frac{(\text{Engine Power} - \dot{E}_{H_2} - W_{\text{comp}})\text{Diesel Fuel Energy}}{100\%} \quad (5.2)
\]
These ideal assumptions are clearly not practical, with the efficiency of the hydrogen generation system being highly dependent on individual components. For example, automotive alternators only have efficiencies of about 55%, which is acceptable, given their benefits, as electrical demands in vehicles are relatively low, while DC generators used for hybrid electric cars are about 95% efficient [100]. Hydrogen generation by traditional (alkaline) electrolysis is about 70% efficient, while advancements in this field including novel catalyst materials and polymer electrolysis membrane (PEM) promise further efficiency increases in the near future [101]. Isentropic compression generates large temperature rises, resulting in heat loss and therefore inefficiencies.

Column i) calculates the total efficiency of the hydrogen generation and compression system required to achieve the same total engine efficiency as the reference case without hydrogen (A.0), and is depicted in Figure 5-7.

\[
\left( \dot{E}_{H2} + W_{comp} \right) / \eta_{H2,gen} = \eta_{ideal[A.0]} * Diesel \ Fuel \ Energy - Engine \ Power \quad (5.3)
\]
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<th>Fuel energy (H2)</th>
<th>Fuel energy rate (total)</th>
<th>Indicated efficiency</th>
<th>Efficiency ideal onboard generation</th>
<th>Max pressure during injection</th>
<th>Required H2 production efficiency</th>
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</table>
Figure 5-5: Computational Results - Engine power

Figure 5-6: Computational Results – Indicated efficiency
5.4.1. Hydrogen Ingestion

Figure 5-8 and Figure 5-10 depict the average in-cylinder pressure and temperature respectively for various levels of hydrogen ingested into the intake air, which correspond to cases A.0 through A.5 in Table 5-2. For comparability of these cases, the Diesel injection timing and duration is held constant at the same values as the 6%vol hydrogen case presented previously. The experimental data for both the 0% and 6% hydrogen case by Liew et al. [9] are included for reference. It should be noted again that these experimental cases allowed the Diesel injection timing to shift with increasing hydrogen levels according to the ECU. Therefore, the computational 0% hydrogen case is not directly comparable to the experimental 0% hydrogen case, while the 6% hydrogen case includes advancement of the injection timing for both the experimental and computational data.
The computational results in Table 5-2 and Figure 5-5 show that engine power remains practically constant for these cases, as the experimental study held engine output power constant by reducing the amount of Diesel fuel. The reduction in total input energy leads to a significant increase in indicated thermal efficiency, reaching 55% indicated efficiency for the 6% hydrogen case (A.4), as seen in Figure 5-6. Even when considering the energy spent to generate the hydrogen from the engine output, a significant benefit to the overall engine efficiency is observed. Additionally, the reduced amount of Diesel fuel leads to a decrease in carbon dioxide emissions of more than 5% for each 1% of hydrogen ingested.

In Figure 5-8 it is observed, that for the 0% hydrogen case, the advancement of the Diesel injection timing alone is responsible for more than 50% of the additional pressure rise exhibited by the 6% hydrogen case. The remaining pressure rise for the hydrogen cases is due to the accelerated combustion kinetics discussed previously. While the effect of increasing peak pressure with advancement of the injection timing is expected due to the increased evaporation time increasing the premixed combustion phase, these results quantify the relative contributions of the hydrogen enhancement compared to the change in injection timing on the peak pressure. These findings are supported by literature, as for a pure Diesel engine, Agarwal et al. pointed out that the carbon dioxide and unburned hydrocarbon emissions were reduced for advanced start of injection, while increasing brake mean effective pressure (bmeP) and brake thermal efficiency, but only at the cost of significantly increased NOx emissions [102].
Figure 5-8 clearly depicts the effects of delaying the point of ignition as hydrogen concentrations increase, which reduces the overall power output due the area under the pressure curve in the expansion stroke increasing.

Figure 5-8 further shows that, at constant injection timing, even small hydrogen concentrations of 1%vol cause a significant rise in peak pressure, similar to the experimental 6% hydrogen case, while further increases in hydrogen concentrations have only small effects on peak pressure. This is in stark contrast to the experimental results by Liew et al., who found that low hydrogen concentrations of 2 to 3 %vol had only negligible effects on peak pressure, as shown in Figure 5-9.
Figure 5-9: Effect of H2 addition on cylinder pressure, 70% load [9]

Keeping in mind that in the experimental cases the Diesel SOI timing advances with increasing hydrogen intake concentrations, the relative increase in peak pressure for low hydrogen concentrations is still much lower in the experimental cases with little SOI advancement compared to the computational results at the higher, constant SOI advancement. Since advancement of the SOI increases the premixed combustion phase relative to the mixing-controlled combustion phase, this leads to the conclusion that the addition of hydrogen primarily interacts with the premixed combustion phase.

The in-cylinder temperature distributions depicted in Figure B-1 increases slightly with increasing hydrogen concentrations. Also, the phasing of the peak temperature advances closer to TDC, as hydrogen concentrations are increased and the premixed combustion phase becomes more dominant.
Figure 5-10: Average Temperature for various levels of intake ingested hydrogen

5.4.2. Dual-cone hydrogen direct injection

The dual-cone hydrogen direct injection cases, B.1 through B.4, experience a significant reduction in indicated engine power, of up to 16.4% for the 6% hydrogen case, as the hydrogen injection amount is increased. This is due to the fact that hydrogen is injected throughout the Diesel injection event, essentially constituting a retardation of the average fuel injection timing compared to the hydrogen ingestion case.

Additionally, the localized nature of the hydrogen distribution within the Diesel fuel cone, as depicted in Figure B-2, causes an increased ignition delay to be observed in the pressure and temperature plots in Figure 5-11 and Figure 5-12.
These results must be viewed with the consideration that the hydrogen direct injection cases presented here, were, for comparability, not optimized for power output or efficiency. Specifically, the Diesel injection timing was not adjusted to account for any ignition delay. The observation of significant additional ignition delay compared to the hydrogen ingestion case therefore suggests that the direct injection of hydrogen would allow further advancement of the Diesel injection and therefore further increase of the premixed combustion phase and resulting efficiency increases, or that alternatively the same effect could be achieved with a reduced amount of hydrogen.

Across all hydrogen levels depicted in Figure 5-11, a slight reduction in the maximum pressure compared to the intake-ingested hydrogen case is observable, which is due to the delayed ignition timing. With the exception of the increased ignition delay, the amount of hydrogen appears to have negligible effects on the in-cylinder pressure. While the peak average temperature in Figure 5-12 is only slightly reduced due to the ignition delay with increasing hydrogen levels, the average temperature after 20° aTDC is reduced significantly. The in-cylinder temperature distribution for the 1% dual cone case is depicted in the second column of Figure B-1 in the appendix. This case performs nearly identically to the 1% hydrogen ingestion case (A.1) in terms of power output and average temperature. However, the in-cylinder temperature distributions at 10° and 15° aTDC show regions of locally increased temperature compared to the hydrogen ingestion case (A.1).
Figure 5-11: Average Pressure for dual cone direct injected hydrogen

The indicated efficiency for the dual cone cases increases by about 2 to 5% with hydrogen increasing hydrogen levels, which is a significant improvement to the reference case (A.0), but marks a reduction compared to the respective hydrogen ingestion cases. This is due to the reduced power output resultant from the additional ignition delay. Taking into account the energy used for the hydrogen generation, a net efficiency loss is observed at hydrogen levels above 2%. While CO\textsubscript{2} emissions are again reduced due to lower Diesel fuel input, the reduced CO\textsubscript{2} amount for the 6% case (B.4) compared to the corresponding 6% hydrogen ingestion case (A.4) suggests significantly incomplete combustion, which further explains the reduction in power output.
5.4.3. Mixed cone hydrogen direct injection

Cases C.1 through C.4 represent the mixed cone hydrogen direct injection cases with concurrent Diesel/hydrogen injection and constant hydrogen injection timing. As with the dual cone cases, a reduction in engine power is observed, although, with a reduction of 7.14% compared to the baseline case, not to the extend as was observed by the dual cone injector. This can be explained by the wider hydrogen distribution observed in the first depiction of column 2 of Figure B-2. This suggests that a well-mixed hydrogen/Diesel mixture is desirable.
The average pressure traces in Figure 5-13 closely resemble the dual cone case. Again, increased ignition delay with increasing hydrogen levels is observed, and peak pressures are slightly reduced compared the intake ingestion cases (A.1-4), but are at similar levels to the dual cone case. The exception is the 1% hydrogen case (C.1), which shows a notably lower peak pressure than the respective 1% dual cone case (B.1).

Figure 5-13: Average Pressure for mixed cone direct injected hydrogen
The average temperature traces in Figure 5-14 show that the 1% hydrogen case actually exhibits the highest peak average temperature. However, peak average temperature occurs later in the expansion stroke at the 1-2% hydrogen levels when compared to the respective dual cone cases. The reason for this is again explained by the larger hydrogen distribution area compared to the dual cone case, which leads to more evenly distributed local hydrogen concentrations and therefore an increased ignition delay throughout the spray cone. Corresponding observations can be made from column 3 of Figure B-1, which shows significantly reduced temperatures up to a crank angle of 15°, and a large high temperature pocket forming in the vicinity of the spray cone at 30° CA.

At 6% hydrogen, case C.4. displays an indicated efficiency of 52.3%. Even under consideration of the energy spent to generate and compress the hydrogen, a net benefit can be achieved in all mixed cone cases under the ideal assumptions of the hydrogen generation system. Under the presented conditions and injection parameters, the mixed cone injector appears more efficient than the dual cone case, keeping in mind that the Diesel injection timing was not optimized for either injector case.
5.4.4. Effect of reduced hydrogen injection duration

In cases C.1 and C.5 through C.7 the effects in hydrogen injection duration are investigated. While the previously discussed cases suggest that engine efficiency generally improves with increasing hydrogen levels, the objective of this research is not to replace Diesel with hydrogen, but to utilize hydrogen solely as a pilot fuel to improve the Diesel combustion. Therefore, a hydrogen enhancement level of 1% was chosen for the remaining cases.
The results tabulated in Table 5-2 show that engine power increases as the hydrogen injection duration is reduced, producing up to 2.27% more power when the hydrogen injection duration is reduced from 29.5 °CA to 5° CA. This results in an overall increase in indicated engine efficiency, since fuel energy input is held constant between these cases. The maximum indicated efficiency increases to 45.23%, compared to the 42.66% of the reference case without hydrogen (A.0).

As the hydrogen injection duration is reduced, the injection event ends prior to the maximum cylinder pressure occurring, meaning that the hydrogen requires less compression to maintain the injection pressure ratio, leading to an ideal engine efficiency considering on-board hydrogen generation of 44.31%.

The average pressure traces for these cases are depicted in Figure 5-15. For hydrogen injection durations of 10° CA and 15° CA, the pressure traces are nearly identical. At very long and very short hydrogen injection timings, the maximum pressure is markedly reduced. In the 5° CA injection duration, the pressure remains very slightly elevated during the expansion stroke compared to the other cases, explaining higher power output of this case.
Figure 5-15: Effects of reduced hydrogen injection duration on pressure

As observed in Figure 5-16, the cases of peak pressure (C.5. and C.6) achieve their peak temperatures earlier, while both very long and very short hydrogen injection result in a slight increase in peak average temperature and temperatures remain elevated throughout the expansion stroke. This increased power production along with the reduced peak pressure may be explained by the elevated hydrogen concentrations in the injection plume depicted in Column 3 of Figure B-2. In fact, the hydrogen injection stops prior to the ignition of the fuel. Column 4 of Figure B-1 shows relatively low temperatures throughout the cylinder until 10 °CA compared to the other cases, after which large high temperature regions begin occurring.
5.4.5. Effects of advanced hydrogen injection timing

Cases C.8 through C.11 explore the advancement of the hydrogen injection timing by 5° and 10° CA prior to the start of the Diesel injection for hydrogen injection durations of 5° and 10° CA. As shown in Table 5-2, the performance these cases in terms of engine power output and engine efficiency are nearly identical to the cases of reduced hydrogen injection duration, meaning that the advancement of the hydrogen injection timing has only marginal effects on the engine performance. Figure 5-17 shows that the average pressure remains nearly constant between these cases throughout the engine cycle.

Figure 5-16: Effects of reduced hydrogen injection duration on temperature
Similarly, the average temperatures in Figure 5-18 show nearly identical peak values. Only case C.9, in which the hydrogen injection event ends as the Diesel injection begins, shows a notable separation between the premixed and the mixing controlled combustion phase, as observed by the two distinct peaks in the temperature profile.

The hydrogen distribution depicted in column 4 of Figure B-2 is notable, as unlike the other cases a large region of hydrogen exists near the injector location at -5 °CA. Owing to its low
density and small injected mass, the hydrogen exhibits poor penetration into the much denser compressed air in the cylinder compared to the Diesel injection spray. The hydrogen is injected prior to the Diesel injection, forming a plume near the injector. The Diesel spray then penetrates this hydrogen plume, entraining some, but not all, of the hydrogen.

Figure 5-18: Effects of early hydrogen injection on temperature
5.5. Conclusions

The effects of hydrogen enhancement in Diesel engines were computationally studied for both, hydrogen ingested into the intake air, and for hydrogen directly injected into the cylinder of a compression ignition engine at various hydrogen enhancement levels.

It was found that increasing levels of hydrogen enhancement provide a net benefit to indicated engine efficiency, allowing for a proportionally larger reduction in the Diesel fuel used, compared to the hydrogen energy it is replaced with. The results show that hydrogen delays the ignition of the fuel charge, thus allowing for advancement of the Diesel injection timing and consequently shifting the combustion from the mixing controlled phase to the premixed combustion phase. This effect is further enhanced by the increase in combustion kinetics shown in the previous chapter. These combined effects result in a closer approximation of the thermodynamically more efficient Otto cycle.

The hydrogen ingestion case showed a maximum indicated efficiency of 55% at a hydrogen enhancement level of 6% by volume of the intake air. At the same hydrogen level, direct injection through a mixed nozzle injector produced a 52.3% indicated efficiency without optimization of the Diesel injection timing. This marks a significant increase compared to the reference case without hydrogen, which produced an indicated efficiency of 42.66%.

A reduction of the hydrogen injection slightly improved the engine efficiency due to the hydrogen having little effect late in the combustion, while early injection of the hydrogen
provided no significant advantage due to the decreased entrainment of the hydrogen by the Diesel injection plume.

The results suggest that the additional efficiency gains achieved Diesel combustion enhanced by hydrogen pilot fuels may be theoretically enough to produce hydrogen from the engine power without detrimental impacts on the engine efficiency and thus reduce carbon dioxide emissions, and/or potentially even increase engine efficiency in an optimized engine.

5.6. Further research

The research presented in this dissertation is only meant to lay the foundation for further research on the possibilities and opportunities of hydrogen-enhanced combustion. The results presented here have yet to be experimentally validated. A full optimization of the hydrogen direct injection scheme, particularly with respect to Diesel injection timing is necessary to determine to its full benefits and to determine if the additional complexity of hydrogen direct injection warrants its use over hydrogen ingestion. Further, a study regarding emissions, in particular with respect to the nitrogen oxides is suggested, as no NOx model was implemented in the computational model presented here.

Additionally, the production of hydrogen through electrolysis of water also produces oxygen, which could also be directed into the engine for additional benefits in volumetric efficiency and combustion performance. Finally, the concept of hydrogen enhanced combustion is not limited to compression ignition engines, as the delay in ignition timing observed in this study could also potentially be applied to gasoline direct injection (GDI) engines to increase compression ratio without knocking.
References


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Appendix A
Chemical Kinetic Mechanism Data

Table A-1: Model M3 Coefficients

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Note: data listed in KIVA input units of mole, cm, s
# Table A-2: Model M4 Coefficients

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<tr>
<td>M4.28</td>
<td>o2+co=&lt;&gt;o+co2</td>
<td>5.00E+12</td>
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<td>47800.0</td>
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<td>M4.29</td>
<td>ho2+co=&lt;&gt;oh+co2</td>
<td>9.52E+13</td>
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<td>23600.0</td>
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<td>M4.30</td>
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<td>5.56E+10</td>
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<td>-76.5</td>
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<td>M4.31</td>
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<td>M4.32</td>
<td>hco+o2=ho2+co</td>
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<td>M4.33</td>
<td>hco+m=h+co+m</td>
<td>1.59E+18</td>
<td>0.9</td>
<td>56712.3</td>
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<td>M4.34</td>
<td>ch3+ch3o=ch4+ch2o</td>
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<td>1.20E+14</td>
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<td>960.0</td>
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<td>M4.36</td>
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<td>M4.37</td>
<td>c2h3+o2=ch2o+hco</td>
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<td>M4.38</td>
<td>c2h3+hco=c2h4+co</td>
<td>6.03E+13</td>
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<td>M4.39</td>
<td>c2h5+o2=c2h4+ho2</td>
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<td>M4.45</td>
<td>ch4+ho2=ch3+h2o2</td>
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<td>M4.46</td>
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<td>M4.47</td>
<td>c3h6=c2h3+ch3</td>
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<td>M4.49</td>
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<td>M4.57</td>
<td>c2h3+c2h3=c2h2+c2h4</td>
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<td>M4.69</td>
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<td>M4.70</td>
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<td>Rate Constant</td>
<td>T (K)</td>
<td>A (cm^3 mol^-1 s^-1)</td>
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<td>M4.71 hco + o = h + co2</td>
<td>3.00E+13</td>
<td>0.0</td>
<td>0.0</td>
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<td>M4.72 hco + ho2 = co2 + oh + h</td>
<td>3.00E+13</td>
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<td>M4.73 c2h6 + ch3 = c2h5 + ch4</td>
<td>1.51E-07</td>
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<td>M4.74 c2h6 + h = c2h5 + h2</td>
<td>5.37E+02</td>
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<td>9.72E+02</td>
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<td>M4.75 c2h6 + oh = c2h5 + h2o</td>
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<td>M4.76 c2h6 + o = c2h5 + oh</td>
<td>1.13E+14</td>
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<td>M4.77 ch3 + ch3 (+m) = c2h6 (+m)</td>
<td>7.37E+16</td>
<td>-1.2</td>
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<td>1.70500E+03</td>
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<td>TROE centering: 0.405</td>
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<td>M4.78 c2h6 + o2 = c2h5 + ho2</td>
<td>4.00E+13</td>
<td>0.0</td>
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<td>Reverse Arrhenius coefficients:</td>
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<td>0.0</td>
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<td>M4.79 c2h6 + ho2 = c2h5 + h2o2</td>
<td>1.70E+13</td>
<td>0.0</td>
<td>20460.0</td>
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<td>1.07E+11</td>
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<tr>
<td>M4.80 c2h6 + c2h4 = c2h5 + c2h5</td>
<td>5.00E+11</td>
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<td>M4.81 c2h6 + m = c2h5 + h + m</td>
<td>8.85E+20</td>
<td>-1.2</td>
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<td>1.15E+13</td>
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<td>M4.82 c2h6 + ch2 = c2h5 + ch3</td>
<td>2.20E+13</td>
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<td>M4.83 c2h6 + ch3o2 = c2h5 + ch3o2h</td>
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<td>M4.84 c3h6 + c2h5 = c3h5 + c2h6</td>
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<td>M4.85 c3h5 + c2h5 = c2h6 + c3h4</td>
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<td>M4.88</td>
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<td>ch2co+h=ch3+co</td>
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<td>M4.92</td>
<td>ch2co(+m)=ch2+co(+m)</td>
<td>3.00E+14</td>
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<td>70980.0</td>
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</table>

Low pressure limit: 3.60000E+15 0.00000E+00 5.92700E+04

| M4.93  | c3h6+o=ch2co+ch3+h  | 2.50E+07 | 1.8 | 76.0    |
| M4.94  | ch2cho=ch2co+h      | 3.09E+15 | -0.3 | 50820.0 |
| M4.95  | ch3+o2+m=ch3o2+m    | 5.44E+25 | -3.3 | 0.0     |
| M4.96  | ch3o2+ch3=ch3o+ch3o | 2.41E+12 | 0.0 | 0.0     |
| M4.97  | ch3o2+o=ch3o+o2     | 3.61E+13 | 0.0 | 0.0     |
| M4.98  | ch3o2+h=ch3o+oh     | 9.64E+13 | 0.0 | 0.0     |
| M4.99  | ch3+oh=ch3+oh       | 1.00E+14 | 0.0 | 0.0     |
| M4.100 | ch3+o=ch2o+h        | 8.00E+13 | 0.0 | 0.0     |
| M4.101 | ch3+o2=ch3o+o       | 2.00E+18 | -1.6 | 29210.0 |

Reverse Arrhenius coefficients: 3.58E+18 -1.6 -1631.0

| M4.102 | ch3+h(+m)=ch4(+m)  | 2.14E+15 | -0.4 | 0.0 |

Low pressure limit: 3.31E+30 -4.00E+00 2.11E+03

TROE centering: 1.00E+15 1.00E+15 4.00E+01

h2 Enhanced by 2.00
h2o Enhanced by 5.00
c0 Enhanced by 2.00
c02 Enhanced by 3.00

| M4.103 | ch3o2h=ch3o+oh     | 6.31E+14 | 0.0 | 42300.0 |
| M4.104 | ch3o2+ch2=ch3o2h+hco | 1.99E+12 | 0.0 | 11670.0 |
| M4.105 | c2h4+ch3o2=c2h3+ch3o2h | 1.13E+13 | 0.0 | 30430.0 |
| M4.106 | ch4+ch3o2=ch3+ch3o2h | 1.81E+11 | 0.0 | 18480.0 |
| M4.107 | ch3o2+ho2=ch3o2h+o2 | 1.75E+10 | 0.0 | -3275.0 |
| M4.108 | oh+ho2=h2o+o2      | 7.50E+12 | 0.0 | 0.0     |
| M4.109 | o+oh=2+h           | 4.00E+14 | -0.5 | 0.0     |
| M4.110 | h+ho2=h2o+o2       | 1.70E+14 | 0.0 | 875.0   |
| M4.111 | oh+oh=o+h2o        | 6.00E+08 | 1.3 | 0.0     |
| M4.112 | h+o2(+m)=ho2(+m)   | 1.48E+12 | 0.6 | 0.0     |

Low pressure limit: 3.50000E+16 -4.10000E-01 -1.11600E+03

TROE centering: 5.00000E-01 1.00000E-30 1.00000E+30

h2 Enhanced by 2.00
h2o Enhanced by 12.00
c0 Enhanced by 1.90

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<td>\text{oh}+\text{oh}(+\text{m})=\text{h}_2\text{o}_2(\pm\text{m})</td>
<td>1.24\times10^{14}</td>
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<td>Low pressure limit:</td>
<td>3.04100\times10^{30}</td>
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<td>TROE centering: 0.47</td>
<td>1.00000\times10^{02}</td>
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<td>M4.114</td>
<td>\text{h}_2\text{o}_2+\text{h}=\text{ho}_2+\text{h}_2</td>
<td>1.98\times10^{06}</td>
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<td>M4.115</td>
<td>\text{h}_2\text{o}_2+\text{h}=\text{oh}+\text{h}_2o</td>
<td>3.07\times10^{13}</td>
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<td>M4.116</td>
<td>\text{h}_2\text{o}_2+o=\text{oh}+\text{ho}_2</td>
<td>9.55\times10^{06}</td>
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<td>M4.117</td>
<td>\text{h}_2\text{o}_2+\text{o}=\text{h}_2\text{o}+\text{ho}_2</td>
<td>2.40\times10^{00}</td>
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<td>M4.118</td>
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<td>1.17\times10^{09}</td>
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<td>M4.119</td>
<td>\text{ho}_2+\text{ho}_2=\text{h}_2\text{o}_2+\text{o}_2</td>
<td>3.00\times10^{12}</td>
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Note: units: A = mole-cm-sec-K and E = cal/mol

### Table A-3: Model M5 Coefficients

<p>|   | \text{h}+\text{o}_2=\text{oh}+\text{o} | 3.52\times10^{16} | -0.7 | 17070.0 |
| M5.109 | \text{h}_2+\text{o}=\text{oh}+\text{h} | 5.06\times10^{04} | 2.7 | 6286.0 |
| M5.110 | \text{h}_2+\text{oh}=\text{h}_2\text{o}+\text{h} | 1.17\times10^{09} | 1.3 | 3633.0 |
| M5.111 | \text{h}_2\text{o}+\text{o}=\text{oh}+\text{oh} | 7.60\times10^{00} | 3.8 | 12760.0 |
| M5.112 | \text{h}+\text{h}+\text{m}=\text{h}_2+\text{m} | 1.30\times10^{18} | -1.0 | 0.0 |
|   | \text{h}_2 \text{ Enhanced by} | 2.5 |
|   | \text{h}_2\text{o} \text{ Enhanced by} | 12 |
|   | \text{c}_0 \text{ Enhanced by} | 1. |
|   | \text{co}_2 \text{ Enhanced by} | 3.8 |
| M5.113 | \text{h}+\text{o}+\text{m}=\text{h}_2\text{o}+\text{m} | 4.00\times10^{22} | -2.0 | 0.0 |
|   | \text{h}_2 \text{ Enhanced by} | 2.50\times10^{00} |
|   | \text{h}_2\text{o} \text{ Enhanced by} | 1.20\times10^{01} |
|   | \text{c}_0 \text{ Enhanced by} | 1.90\times10^{00} |
|   | \text{co}_2 \text{ Enhanced by} | 3.80\times10^{00} |
| M5.114 | \text{o}+\text{oh}=\text{o}_2+\text{m} | 6.17\times10^{15} | -0.5 | 0.0 |
|   | \text{h}_2 \text{ Enhanced by} | 2.50\times10^{00} |
|   | \text{h}_2\text{o} \text{ Enhanced by} | 1.20\times10^{01} |
|   | \text{c}_0 \text{ Enhanced by} | 1.90\times10^{00} |
|   | \text{co}_2 \text{ Enhanced by} | 3.80\times10^{00} |
| M5.115 | \text{h}+\text{oh}+\text{m}=\text{oh}+\text{m} | 4.71\times10^{18} | -1.0 | 0.0 |
|   | \text{h}_2 \text{ Enhanced by} | 2.50\times10^{00} |</p>
<table>
<thead>
<tr>
<th>Equation</th>
<th>Reaction</th>
<th>A (molec-cm-sec-K)</th>
<th>E (cal/mol)</th>
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<td>1.00000E+15</td>
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<td>M5.118</td>
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<td>co Enhanced by</td>
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</table>

Note: units: A = mole-cm-sec-K and E = cal/mol
Appendix B
In-cylinder visualizations

Figure B-1: In-cylinder temperature variation
Figure B-2: In-cylinder hydrogen (mfrach2) and Diesel (mfrac1) fuel mass fraction distributions