MODELING INJECTION AND IGNITION IN DIRECT INJECTION
NATURAL GAS ENGINES

by

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Abstract

With increasing concerns about the harmful effects of conventional liquid fossil fuel emissions, natural gas has become a very attractive alternative fuel to power prime movers and stationary energy conversion devices. This research studies the injection and ignition numerically for natural gas (mainly methane) as a fuel applied to diesel engine.

Natural gas injector and glow plug ignition enhancement are two of the most technical difficulties for direct injection natural gas engine design. This thesis models the natural gas injector, and studies the characteristics of the internal flow in the injector and natural gas jet in the combustion chamber during the injection process. The poppet valve model and pintle valve model are the first reported models to simulate the natural gas injector to improve the traditional velocity and pressure boundary conditions.

This thesis also successfully models the glow plug assisted natural gas ignition and combustion processes by developing a glow plug discretized model and a novel virtual gas sub-layer model. Glow plug discretized model can describe the transient heat transfer, and adequately represents the thin layers of heat penetration and the local temperature difference due to the cold gas jet impingement. The virtual gas sub-layer model considers complicated physical processes, such as chemical reaction, heat conduction, and mass diffusion within the virtual sub-layers without significantly increasing computational time and load.

KIVA-3V CFD code was chosen to simulate the fluid flow. Since the KIVA-3V is designed specifically for engine research application with conventional liquid fuels, many modifications have been implemented to facilitate this research.
Acknowledgments

I would like to take this opportunity to express my sincerest thanks and appreciation to my supervisor, Professor James Wallace, for his invaluable guidance, consistent encouragement, patience and kindness, and financial support during my five years study at University of Toronto. I would also like to extend my gratitude to Professor Pierre Sullivan, Professor Dongqing Li, and Professor Markus Bussmann, who offered me valuable advice during the meetings with me.

Also, I would like to acknowledge the contributions to and Mark Fabbroni and David Wager for their experimental work and the valuable data, their explanations and discussions, and to those who previously worked in the lab, especially Paul Selanki, Alvin Cheung, Eric Brombacher, and Vito Abate for laying the foundation for this project.

It was my pleasure to work in a great lab with wonderful colleagues and friends. Thank you for your help, Hannu Jääskeläinen, Mark Fabbroni, Deokkyu Park, David Wager, Bradley Bretecher. I wish them the best in their future life.

Finally I want to express my heartfelt thanks to my family - my beloved wife and two lovely sons, to whom this thesis is dedicated. They are always behind me to provide their endless love, strongest support and encouragement to help me overcome the difficulties. Thank you, mom, dad, and my two sisters, thanks for your love and encouragement.
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Nomenclature

Symbols:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Cross section area</td>
</tr>
<tr>
<td>$A_s$</td>
<td>Surface area of the glow plug</td>
</tr>
<tr>
<td>$A_c$</td>
<td>Input for the swirl profile, determines the amplitude of the swirl velocity</td>
</tr>
<tr>
<td>$A_{br}$</td>
<td>Backward coefficient for reaction $r$</td>
</tr>
<tr>
<td>$A_f$</td>
<td>Forward coefficient for reaction $r$</td>
</tr>
<tr>
<td>$a_{isp,r}$</td>
<td>Integer stoichiometric coefficient for reaction $r$</td>
</tr>
<tr>
<td>$a_{isp-r}$</td>
<td>Empirical order of the reaction</td>
</tr>
<tr>
<td>$A_n$</td>
<td>Nozzle orifice area</td>
</tr>
<tr>
<td>$B_i$</td>
<td>Biot number</td>
</tr>
<tr>
<td>$b_{isp,r}$</td>
<td>Integer stoichiometric coefficient for reaction $r$</td>
</tr>
<tr>
<td>$b_{isp-r}$</td>
<td>Empirical order of the reaction</td>
</tr>
<tr>
<td>$c_1$</td>
<td>Constant for built-in turbulence k-e equations in KIVA-3V code</td>
</tr>
<tr>
<td>$c_2$</td>
<td>Constant for built-in turbulence k-e equations in KIVA-3V code</td>
</tr>
<tr>
<td>$c_2$</td>
<td>System constant including effects of geometry, gas properties and flow pattern</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Glow plug specific heat</td>
</tr>
<tr>
<td>$C_{pgas}$</td>
<td>Heat capacity of the surrounding gas at constant pressure</td>
</tr>
<tr>
<td>$c_v$</td>
<td>Heat capacity at constant volume</td>
</tr>
<tr>
<td>$D$</td>
<td>Diameter of the glow plug, $[m]$</td>
</tr>
<tr>
<td>$D_{isp}$</td>
<td>Mass diffusion coefficient for species $isp$, also called the mass diffusivity, $[m^2/s]$</td>
</tr>
<tr>
<td>$dX_{isp}/dx$</td>
<td>Mass fraction gradient for species $isp$</td>
</tr>
<tr>
<td>$E$</td>
<td>Internal energy</td>
</tr>
<tr>
<td>$E/R$</td>
<td>Activation temperature, $(E/R = 25000 \text{ K for methane})$</td>
</tr>
<tr>
<td>$E_{br}$</td>
<td>Backward activation temperature for reaction $r$, $[K]$</td>
</tr>
<tr>
<td>$E_f$</td>
<td>Forward activation temperature for reaction $r$, $[K]$</td>
</tr>
</tbody>
</table>
$Fo$ - Fourier number

$G$ - Mass flow rate

$G^{*}$ - Theoretical mass flow rate of 1-D isentropic flow

$h$ - Convective heat transfer coefficient

$h_{isp}$ - Specific enthalpy for species $isp$

$I$ - Current [$A$]

$i$ - Index of the sub-layers

$i/i+1$ - Subscript for boundary between sub-layer $i$ and sub-layer $i+1$

$isp$ - The index of species involved in the reaction $r$

$J_{isp}$ - Mass diffusion flux for species $isp$, [$kg/m^2-s$]

$j_{0}, j_{1}, j_{2}$ - Bessel function of the first kind of order 0, 1, and 2.

$k$ - Thermal conductivity

$k_{br}$ - Backward rate coefficients for reaction $r$

$k_{fr}$ - Forward rate coefficients for reaction $r$

$k_{gas}$ - Gas thermal conductivity

$M$ - Mach number

$\cdot m$ - Theoretical mass flow rate from nozzle

$\cdot M_{n}$ - Momentum injection rate at the nozzle

$n$ - Global reaction order, ($n \approx 1.7$ for methane)

$Nu$ - Nusselt number

$P$ - Charge air pressure

$P_{h}$ - Pressure at high pressure reservoir

$P_{0}$ - Upstream gas pressure

$P_{BDC}$ - Pressure at BDC

$P_{ex}$ - Pressure at low pressure reservoir

$P_{max}$ - Peak pressure in cylinder

$Pr$ - Prandtl number

$P_{s}$ - Input for the swirl profile, determines the shape of the swirl velocity profile, $0 < Ps < 3.84$.

$q$ - Heat flux

$q_{\cdot}$ - Conduction heat transfer rate from the glow plug surface

$q$ - Negative of the heat of reaction $r$ at absolute zero

$q$ - Volumetric energy released from chemical reaction

$q_{chem}$ - Volumetric energy release from all the chemical reactions

$R$ - Gas constant
\( R \) - Thermal resistance (K/W)
\( R_a \) - Rayleigh number
\( R_e \) - Reynolds number
\( r \) - Radius coordinate in cylindrical coordinate system
\( r \) - The index of chemical reaction
\( T \) - Jet dynamic temperature
\( T_{\text{film}} \) - Film temperature of the Glow plug
\( T_s \) - Surface temperature of the Glow plug
\( t \) - Time after start of injection
\( T_{\infty} \) - Surrounding air temperature
\( T_0 \) - Temperature at high pressure reservoir
\( T_0 \) - Upstream gas temperature
\( T_e \) - Charge air temperature
\( T_{\text{ex}} \) - Temperature at low pressure reservoir
\( T_{\text{gas}} \) - Temperature of the surrounding gaseous cell
\( T_{\text{gp}} \) - Surface temperature of the glow plug cell
\( T_i \) - Initial temperature of the glow plug
\( T_{\text{ign}} \) - Auto ignition temperature in mixture
\( T_{\text{inj}} \) - Injection temperature
\( T_n \) - Injector gas temperature
\( T_s \) - Surface temperature of the glow plug
\( T_{\text{surrr}} \) - Surrounding temperature
\( T_w \) - Hot surface temperature
\( u_{(isp)} \) - Specific internal energy for species \( isp \)
\( V \) - Velocity, [m/s]
\( V \) - Voltage, [V]
\( V \) - Volume, [m³]
\( v_{(isp)} \) - Specific volume for species \( isp \)
\( V(r) \) - Swirl velocity at radius \( r \)
\( V_{\text{sac}} \) - Sac volume of the injector
\( W_{isp} \) - Molecular weight of the species \( isp \) involved in the reaction \( r \)
\( X \) - Species fraction
\( X_{(isp)} \) - Mass fraction for species \( isp \)
\( z \) - Height coordinate in cylindrical coordinate system
\( Z_t \) - Jet penetration
\( \alpha \) - Thermal diffusivity of the glow plug \([m^2/s]\), \( \alpha = \frac{k}{\rho \cdot c_p} \)

\( \alpha_{\text{gas}} \) - Thermal diffusivity of the surrounding gas, \( \alpha_{\text{gas}} = \frac{k_{\text{gas}}}{(\rho_{\text{gas}} \cdot C_{p_{\text{gas}}})} \)

\( \chi_{isp} \) - Represents one mole of species \( isp \)

\( (\Delta h^0_{isp})_{isp} \) - Heat of formation of species \( isp \) at absolute zero

\( \delta \) - Heat penetration thickness

\( \delta_{\text{gas}} \) - Thickness of the gaseous cell

\( \varepsilon \) - Emissivity of the glow plug

\( \phi \) - Fuel/Air equivalence ratio

\( \Gamma \) - Constant for the turbulent jet issued from the nozzle

\( \Gamma \) - Dimensionless number obtained from their experiment

\( \gamma \) - Ratio of specific heats

\( \mu \) - Viscosity and

\( \nu \) - Kinematic viscosity

\( \theta \) - Angular coordinate in cylindrical coordinate system

\( \theta \) - Crank angle position

\( \rho \) - Density of the gases

\( \rho \) - Glow plug density

\( \rho_{a} \) - Chamber gas density

\( \rho_{\text{gas}} \) - Density of the surrounding gas

\( \rho_{isp} \) - Density of the species \( isp \) involved in the reaction \( r \)

\( \sigma \) - Stefan-Boltzmann constant, \( 5.670 \times 10^{-8} \) W·m⁻²·K⁻⁴

\( \tau_i \) - Total ignition delay \([\text{ms}]\)

\( \tau_{tf} \) - Penetration delay \([\text{ms}]\)

\( \cdot \) - Speed of the kinetic reaction \( r \)

\( \cdot \) - Chemical reaction speed for reaction \( r \) in sub-layer \( i \).

\( \zeta_{br} \) - Backward coefficient for reaction \( r \)

\( \zeta_{fr} \) - Forward coefficient for reaction \( r \)

\( \frac{\partial E_{\text{diff}}}{\partial t} \) - Total energy change rate for all species due to the mass diffusion

\( \frac{\partial E_{\text{diff}(isp)}}{\partial t} \) - Energy change rate for species \( isp \) due to the mass diffusion

\( \frac{\partial m_{\text{isp}}}{\partial t} \) - Mass change for species \( isp \) due to all of the chemical reactions

\( \frac{\partial m_{\text{all}}}{\partial t} \) - Total mass change rate for all species due to the mass diffusion
\[ \frac{\partial m_{isp}}{\partial t} \] - Mass change rate for species \( isp \) due to the mass diffusion

\[ \frac{\partial m_{isp}}{\partial t} \] - Mass change for species \( isp \) due to the chemical reaction \( r \)

**Abbreviations:**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATDC</td>
<td>After Top Dead Center Piston Position</td>
</tr>
<tr>
<td>BC</td>
<td>Boundary condition</td>
</tr>
<tr>
<td>BDC</td>
<td>Bottom Dead Center Piston Position</td>
</tr>
<tr>
<td>BMEP</td>
<td>Brake Mean Effective Pressure</td>
</tr>
<tr>
<td>BTDC</td>
<td>Before Top Dead Center Piston Position</td>
</tr>
<tr>
<td>CA</td>
<td>Crank Angle</td>
</tr>
<tr>
<td>CAD</td>
<td>Crank Angle Degree</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CFR</td>
<td>Cooperative Fuel Research</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon Monoxide</td>
</tr>
<tr>
<td>DI</td>
<td>Direct Injection</td>
</tr>
<tr>
<td>DING</td>
<td>Direct Injection Natural Gas</td>
</tr>
<tr>
<td>ERDL</td>
<td>Engine Research and Development Laboratory</td>
</tr>
<tr>
<td>GP</td>
<td>Glow Plug</td>
</tr>
<tr>
<td>ICCD</td>
<td>Intensified Charge Coupled Device</td>
</tr>
<tr>
<td>LHV</td>
<td>Low Heating Value</td>
</tr>
<tr>
<td>MFI</td>
<td>Mixing Fuel Injection</td>
</tr>
<tr>
<td>NG</td>
<td>Natural Gas</td>
</tr>
<tr>
<td>NO(_x)</td>
<td>Oxides of Nitrogen (e.g. NO, NO(_2))</td>
</tr>
<tr>
<td>PFI</td>
<td>Pilot Fuel Injection</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate Matter</td>
</tr>
<tr>
<td>RPM</td>
<td>Revolutions Per Minute</td>
</tr>
<tr>
<td>SI</td>
<td>Spark Ignition</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of Injection</td>
</tr>
<tr>
<td>TDC</td>
<td>Top Dead Center Piston Position</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Natural Gas Fueled Engines

Interest in developing alternative fuel technologies for vehicular use and power generation began in the 1970s in response to the energy crisis and the realization that the world’s crude oil supply is finite [Nichols, 1993]. As crude oil prices have increased in recent years, more research has focused on alternative fuels, such as bio-diesels and natural gas. Currently natural gas is less expensive than diesel fuel*, as well as being domestically available with an established (but limited in scope) infrastructure for refueling purposes.

Two types of internal combustion engines are in widespread use: spark ignition (SI) and compression ignition (CI) engines. The former dominates the passenger car market. In the SI engine, a homogeneous mixture of air and fuel, typically gasoline, is taken into the engine, compressed and ignited by a spark. In the CI engine, only air is taken into the engine and

* Although this is due to the absence of road tax on natural gas at present in many countries including Canada.
compressed to a higher temperature. Fuel, typically diesel fuel, is injected into the hot air where it is vaporized, mixed with air and spontaneously ignites. CI engines dominate the heavy duty engine market due to their higher efficiency.

The technology for natural gas fueled SI engines is straightforward and widely available. The technology for utilizing natural gas in a compression ignition engine - the direct injection natural gas (DING) engine – is still under development, however.

The key difficulty is that natural gas does not spontaneously ignite in the time available when injected into typical engine cylinder conditions of temperature. Thus, some form of ignition assist is necessary to achieve ignition in practical DING engines. The motivation for this thesis is to establish a physical understanding of one form assisted ignition – ignition by hot surface.

1.1.1 The Benefits of Natural Gas as a Fuel for Engines

With increasing concerns about the harmful effects of conventional fossil fuel emissions, such as those from gasoline and diesel fuel, natural gas has become a very attractive alternative fuel to power prime movers and stationary energy conversion devices [Richards, 1992]. For reciprocating engines, natural gas has emerged to be a promising alternative fuel due to its lower cost, clean burning quality. The emissions of particulate (PM), nitrogen oxides (NOx), and carbon oxides could be significantly reduced for natural gas compared to traditional hydrocarbon fuels [Papageorgakis et al., 1996].

Using natural gas in a vehicle is not as convenient as traditional liquid fuels. To be stored on board, it must be compressed or liquefied, and the safety issues have been solved
satisfactorily. Natural gas fueling does add some parasitic losses that are not present in a conventional diesel engine. This results from the need to compress low pressure natural gas from an onboard tank to a high pressure for injection.

1.1.2 The Advantages of a Direct Injection Natural Gas (DING) Engines

Technologies for natural gas applied in homogeneously premixed spark ignition (SI) engines are more mature than those in direct injection (DI) auto-ignition diesel engines. But premixed operation has several drawbacks in terms of engine performance. SI engines generally have 30% lower power output than the same size diesel engine due to detonation-limited brake mean effective pressure (bmeq) capability. SI engines also suffer from 15-25% lower thermal efficiency than the traditional diesel engine due to detonation-limited lower compression ratio and high intake air pumping losses resulting from the need to throttle the intake air pressure at the part load conditions [Willi and Richards, 1994].

Direct Injection Natural Gas (DING) engines have been reported to have a higher thermal efficiency and a higher power output compared to the conventional SI gas engine. Ikeda et al. [1995] found that the eight-cylinder DING engine had 43% higher brake thermal efficiency, and two times the brake mean effective pressure as compared to the conventional spark ignition gas engine. Richards reported that their DING engine had 35% higher power output and 31% higher thermal efficiency than a conventional spark ignition natural gas engine using the 3500 series engines [Richards, 1992]. A comparison of spark ignition and direct injection natural gas engines is summarized in table 1.1.
Table 1.1 Comparison of spark ignition and direct injection natural gas engines

<table>
<thead>
<tr>
<th>Ignition</th>
<th>Spark Ignition</th>
<th>Direct Injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Supply</td>
<td>Homogeneously premixed</td>
<td>High pressure, direct injection auto-ignition</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>Low (8~12)</td>
<td>High (12~24)</td>
</tr>
<tr>
<td>Technology</td>
<td>Mature</td>
<td>Developing</td>
</tr>
<tr>
<td>Thermal Efficiency</td>
<td>15~25% lower</td>
<td>- -</td>
</tr>
<tr>
<td>Power output</td>
<td>30% lower</td>
<td>- -</td>
</tr>
</tbody>
</table>

Because the DING engine avoids detonation limitations by only inducting and compressing fresh air, and injecting gaseous fuel at the time of combustion, the compression ratio can be increased to that of a traditional diesel engine (12~24) as compared to the lower compression ratio of SI gas engine (8~12).

1.2 Features of Natural Gas Fuel and Injection Jet for DING Engines

Compared to conventional liquid fossil fuels, methane, the primary component of natural gas has higher chemical stability which implies difficulties for auto ignition. In this context, high chemical stability refers to a higher spontaneous ignition point and a lower flammability range for natural gas as shown in table 1.2. When it is applied to a direct injection diesel engine application, because its injection features of low temperature after expansion and unfavorable mixing for the jet with the cylinder air as discussed in chapter 4, it will generate a technical challenge for the auto ignition, which is not an issue for liquid fuels at injection.
1.2.1 Chemical Features of Natural Gas Fuel

Methane has a very stable chemical structure compared with higher-chain hydrocarbon bonds of the liquid fuels. Table 1.2 compares the combustion properties of methane with those of other fuels. The high spontaneous ignition point and narrow flammability range for pure methane generates more difficulties to its ignition over a reasonably short time for engine applications (2 ms as a criterion usually used for engine fuel auto ignition delay) [Richards, 1992].

Table 1.2 Fuel combustion properties [Willi and Richards, 1994]

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Diesel</th>
<th>Methanol</th>
<th>Methane</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spontaneous ignition point (K)</td>
<td>589</td>
<td>743</td>
<td>903</td>
<td>--</td>
</tr>
<tr>
<td>Flammability range (% vol in air)</td>
<td>0.6~7</td>
<td>7~36</td>
<td>5~15</td>
<td>4~74</td>
</tr>
<tr>
<td>Ratio of flammability range limits</td>
<td>11</td>
<td>5</td>
<td>3</td>
<td>19</td>
</tr>
<tr>
<td>Ignition temperature (K)*</td>
<td>800</td>
<td>1075</td>
<td>1130</td>
<td>1030</td>
</tr>
<tr>
<td>(2 ms delay for engine application)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1.2.2 Cold Jet Temperature due to the Natural Gas Rapid Expansion

When natural gas is injected from the high pressure injector line to the low pressure diesel engine combustion chamber, the jet undergoes a rapid expansion. Often, because of a choked flow condition the velocity reaches sonic speed at the nozzle exit, further expanding to supersonic at near exit locations (usually generating shock waves) until the flow expands to the back pressure.

* The reference for this row is [Richards, 1992].
The natural gas thermal energy is transformed to high kinetic energy in the nozzle, where temperature of the natural gas jet falls significantly. The dynamic temperature can be expressed as 

\[ \frac{T_{\text{inj}}}{T} = 1 + \frac{\gamma - 1}{2} M^2 \]  

[Liepmann and Roshko, 1957], where \( T_{\text{inj}} \) and \( T \) are the injection temperature and jet dynamic temperature correspondingly, \( \gamma \) is the ratio of the specific heat at constant pressure to the one at constant volume, and \( M \) is the Mach number. For typical engine applications, if the ratio of the injection pressure to engine combustion chamber pressure is 3, the temperature ratio of \( T_{\text{inj}}/T \) can be as low as 1.3, implying a significant temperature drop. This temperature drop effect for natural gas injection has been reported by many researchers [Sun, 1999; Tang, 1997; Li et al., 2005].

1.2.3 Air Entrainment and Unfavorable Mixing of the Natural Gas Jet

When liquid fuel is injected at very high pressure (the cylinder pressure at injection is typically in the range of 50-100 atm, and fuel injection pressure is in the range of 200-1700 atm depending on the engine size and type of combustion system employed), it is broken into very tiny droplets (sizes in the order of 10 \( \mu \text{m} \)) [Heywood, 1988]. The droplets then evaporate and mix with the surrounding air, generating a relatively good fuel air mixture for ignition. Unlike liquid fuels, the natural gas jet entrains air only at its outer boundary, and forms a very thin layer of flammable fuel-air mixture which corresponds to fuel-air equivalence ratio \( \phi \) of 0.5~1.5. Fuel air equivalence ratio is fuel air mass ratio normalized by stoichiometric mixture, i.e., it is a ratio of fuel air mass ratio of a mixture to fuel air mass ratio of a stichiometric mixture, where a stichiometric mixture has a fuel air equivalence ratio of 1. The fuel air equivalence ratio \( \Phi \) can be expressed as:
\[
\Phi = \frac{m_{\text{fuel}} / m_{\text{air}}}{(m_{\text{fuel}} / m_{\text{air}})_{\text{stoich}}},
\]

where: 
- \(m_{\text{fuel}}\) is the mass of fuel; 
- \(m_{\text{air}}\) is the mass of air; 
- suffix \(st\) stands for stoichiometric conditions.

Figure 1.1 shows the fuel air equivalence ratio contour development history [Sun, 1999].

1.2.4 Ignition Difficulties

Methane, which has a higher spontaneous ignition temperature than conventional liquid hydrocarbon fuels, requires unrealistic compression ratios on the order of 29:1 to achieve temperatures at which ignition will occur in a short delay time (usually within 2ms) essential for
efficient engine operation [Fraser, 1988]. This imposes impractical thermal and mechanical loads on the engine. Also the natural gas jet, which has a low temperature because of the high expansion and a thin outer boundary layer in the flammable region because of the unfavorable fuel-air mixing, adds extra difficulties for achieving auto-ignition of the natural gas jet. Thus, natural gas cannot self-ignite under normal engine operations; it requires some form of ignition enhancement to ensure that ignition occurs under a wide range of engine operation conditions at different speeds and loads.

1.3 Ignition Enhancement Methods for DING engines

Ignition enhancement is designed to ensure high energy at a specific location to increase the local temperature of the natural gas fuel-air mixture so the chemical reaction can be enhanced and ignition realized. The following ignition enhancement methods: pilot fuel system, hot surface (glow plug), spark ignition (spark plug), and other methods such like laser ignition and chemical additives as catalyst, are discussed below.

1.3.1 Pilot Fuel System

The pilot fuel system uses pilot fuel having excellent auto ignition quality (e.g. diesel fuel) to first auto ignite, then burn the main fuel. The advantage of this method is reliable ignition with mature technology, and it is now commercially applied to the DING engine. The disadvantage of the pilot fuel system is with the pilot diesel fuel, there is a complicated dual fuel injection system and the necessity of carrying two fuels on a vehicle. Also, diesel fuel generates higher emissions.
There are two different types of pilot fuel systems - Pilot Fuel Injection (PFI) and Mixing Fuel Injection (MFI) [Miyake et al., 1983]. The first injects a pilot fuel (diesel) into the cylinder before injecting the main fuel (natural gas), and the second is to inject the pilot fuel in advance into the natural gas supply, so that the pilot fuel and the main gas fuel are injected together in a mixed form into the cylinder. General speaking, PFI needs a smaller amount of pilot fuel compared to MFI, although it requires a more complicated dual fuel injector. Typically, the amount of pilot fuel required needs to be equivalent to a few percent of the total calorific value of the fuels injected into the cylinder under full load [Miyake et al., 1983].

1.3.2 Spark Ignition (Spark Plug)

The advantage of spark ignition is that it is technically mature and spark plugs are commercially available, but the spark plug lifetime is short for applications which operate continuously such as stationary engines. The biggest disadvantage of spark ignition is that it is hard to achieve stable ignition under all operating conditions due to the very different composition of the mixtures around the spark plug position in different operating states.

1.3.3 Hot Surface (Glow Plug)

The advantage of using a hot surface to assist ignition is lower emissions by avoiding dual fuel combustion. A hot surface assisted ignition system eliminates all disadvantages of dual fuel systems, keeping the injector relatively simple and reliable, and avoids carrying two fuels in a vehicle.
One form of hot surface, a glow plug, is already in widespread use in diesel engines as a cold starting aid. A glow plug is typically a thin pencil shaped heating element that protrudes into a diesel engine combustion chamber.

Figure 1.2 shows a typical glow plug commercially available from NGK Spark Plug Co. Ltd [www.NGK.de]. The detailed structure, dimension, and functional parameters are introduced in section 5.1.1.

Since present glow plugs were only designed for short term operation during the cold start period, continuous operation of an ignition assist device is a very challenging requirement. Glow plug lifetime in the role of continuous ignition assist is still an issue. In anticipation of having glow plugs with adequate lifetimes, much research has been conducted in this field to discover what are the important parameters to reduce ignition delay time. These factors are: glow plug temperature, glow plug number, and glow plug orientation.

A shield surrounding the glow plug has proven to reduce ignition delay time because it holds the surrounding fuel air mixture near the glow plug ensuring effective heat transfer from the hot glow plug to the mixture [Aesoy and Valland, 1996; Fukuda et al., 1993].

Although increasing the glow plug temperature reduces the ignition delay and stabilizes the auto-ignition process, the glow plug requires a temperature as low as possible to prolong its lifetime. This is the main technical difficulty for the glow plug application in the DING engine, and will be an important research motivation of this work.
1.3.4 Other Methods

There are other ignition enhancement methods that are being researched, such as laser ignition and catalyst additives.

Ongoing research into laser ignition is being conducted at several institutes in the US, Europe and Japan for large bore diesel engines. Laser ignition uses a highly-localized energy ($10^{12}\text{W/m}^2$) from a laser to provide instantaneous local high temperature to ignite the gas. Issues remaining include cost, control, stability, and window cleaning for the laser optical passage [Ahrens et al., 2005; Yalin et al., 2005].

Another technique would be to find an effective chemical additive which can be mixed within the natural gas, so that it can dramatically decrease the auto-ignition temperature of the fuel to achieve self-ignition by the normal engine compression ratio. The idea would be similar to the chemical cetane improvers such as hexamethyl nitrate that are widely used in diesel fuel. This method applied to natural gas is not mature yet. To date no effective additive has been found, by which the auto ignition delay time could be reduced to the required level.

From a technical point of view, the glow plug assisted ignition method is a promising direction to develop an ignition assist system for direct injection natural gas engines.

1.4 Parameters that Affect Ignition in a Glow Plug Assisted DING Engine

The glow plug assisted DING engine may have very low emissions. Although it is not mature enough for commercialization, previous work has identified important parameters to reduce ignition delay time. These factors include: glow plug temperature, natural gas
composition, charge air temperature, charge air pressure, and injection conditions and hot surface orientation.

Most research was done with two typical experimental setups: a constant volume combustion bomb, e.g. figure 1.3 from Aesoy and Valland [1996], or a direct injection diesel engine, e.g. figure 1.4 from Ikeda et al. [1995]. The present work is based on the constant volume combustion bomb situation.

![Figure 1.3 Experimental setup of constant volume of combustion bomb](Aesoy, 1996)  
![Figure 1.4 Experimental setup of the direct injection natural gas engine](Ikeda, 1995)

### 1.4.1 Glow Plug Temperature

Previous research on natural gas ignition by a hot surface has shown that the ignition delay of the natural gas was reduced with increased hot surface temperature. But as the hot
surface temperature increases to a higher value, the rate of decrease of ignition delay is reduced as shown in figure 1.5 [Aesoy and Valland, 1996]. To achieve an ignition delay of 2 ms (corresponding to 12 CAD for an engine at 1000 rpm), pure methane needs a hot surface temperature at 1208 K [Willi and Richards, 1994].

Aesoy and Valland [1996] tested the effects of hot surface temperature on ignition delay time using a hot hollow cylinder in a constant volume combustion bomb, through which the natural gas was injected into the bomb (as shown in figure 1.3). As the hot surface temperature was increased, the ignition delay time was reduced (figure 1.5). The composition of the natural gas mixtures tested is shown in table 1.3. Together figure 1.5 and table 1.3 show that decreasing methane concentration and increasing propane concentration decreases ignition delay at a given hot surface temperature. This will be further discussed in the next section.

Figure 1.5 Ignition delay as function of hot surface temperature ($T_w$) for various natural gas mixtures compared to pure methane [Aesoy and Valland, 1996].
Table 1.3 Composition of the test gases in figure 1.5 [Aesoy and Valland, 1996].

<table>
<thead>
<tr>
<th>Test Gas</th>
<th>The Concentration for Gas Components (%)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CH(_4)</td>
<td>C(_2)H(_6)</td>
<td>C(_3)H(_8)</td>
<td>C(_4)+</td>
</tr>
<tr>
<td>Methane (ref.)</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Natural gas A</td>
<td>92.2</td>
<td>5.4</td>
<td>0.3</td>
<td>2.1</td>
</tr>
<tr>
<td>Natural gas B</td>
<td>90.9</td>
<td>5.3</td>
<td>1.8</td>
<td>2.0</td>
</tr>
<tr>
<td>Natural gas C</td>
<td>87.8</td>
<td>5.2</td>
<td>5.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Natural gas D</td>
<td>84.8</td>
<td>5.2</td>
<td>8.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Furthermore, Aesoy and Valland fit their data to a global ignition model in the form of the Arrhenius equation (equation 1.1), and these data showed a good agreement with this equation.

\[
\tau_i = \tau_{if} + C_2 \cdot p^{-n} \cdot \left(\frac{T_w - T_e}{T_w}\right)^2 \cdot e^{E/RT_w} \quad (T_e < T_{ign} < T_w)
\]  

(Equation 1.1)

where:
- \(\tau_i\) total ignition delay [ms]
- \(\tau_{if}\) penetration delay [ms]
- \(p\) charge air pressure [bars]
- \(n\) global reaction order (\(n \approx 1.7\) for methane)
- \(T_w\) surface temperature [K]
- \(T_e\) charge air temperature [K]
- \(T_{ign}\) auto ignition temperature in mixture [K]
- \(C_2\) system constant including effects of geometry, gas properties and flow pattern
- \(E/R\) activation temperature (E/R \(\approx 25000\) K for methane)
The correlations of the experimental results and the ignition model are shown in figure 1.6, and the empirical (Arrhenius) constants are found to be [Aesoy and Valland, 1996]:

\[ E/R \approx 24500 \text{ K for natural gas (85-100\% methane)} \]

\[ n \approx 1.75 \]

Figure 1.6 Arrhenius plot of ignition delay found experimentally for different natural gas mixtures correlated to the ignition model [Aesoy and Valland, 1996].
1.4.2 Natural Gas Composition

As noted earlier, ignition delay is reduced with higher alkane additives, e.g. more propane, less methane. Extensive experiments were done by Aesoy on ignition delay using different natural gas compositions [Aesoy and Valland, 1996]. For higher alkanes, chemical radicals are easier to generate due to lower chemical stability compared to the lower alkanes. Thus, ignition delay is reduced. The temperature reduction by increasing the alkane additives can be as high as a 100 K. This would result in a significant improvement to the glow plug lifetime due to lower thermal stress, although it does not eliminate the need for hot surface assistance.

Aesoy and Valland [1996] studied the effects of natural gas components on ignition delay time in both a constant volume combustion bomb and in a one-cylinder test engine. A glow plug was used for ignition enhancement in the test engine with high pressure direct natural gas injection. As shown in table 1.4 and figure 1.7, higher alkane additives reduce ignition delay time for natural gas in their test engine.
Figure 1.7 Relative ignition temperature of pure two-component gas mixtures of methane added small fractions of ethane, propane, hydrogen and ethane [Aesoy and Valland, 1996]

Table 1.4 Ignition delay for various natural gas mixtures tested in a single-cylinder engine [Aesoy and Valland, 1996]

<table>
<thead>
<tr>
<th>Gas mixture</th>
<th>CH4</th>
<th>C2H6</th>
<th>C3H8</th>
<th>C4+</th>
<th>H2</th>
<th>C2H4</th>
<th>N2</th>
<th>CO2</th>
<th>Glow plug electrical power [W]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>100</td>
<td>0.9</td>
<td>0.3</td>
<td>1.0</td>
<td></td>
<td>1.0</td>
<td></td>
<td>1.0</td>
<td>203</td>
</tr>
<tr>
<td>Natural gas (NG)</td>
<td>91.9</td>
<td>5.9</td>
<td>0.9</td>
<td>0.3</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
<td>1.0</td>
<td>3.1</td>
</tr>
<tr>
<td>NG + 3.5% Ethane</td>
<td>88.3</td>
<td>9.5</td>
<td>0.9</td>
<td>0.3</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
<td>1.0</td>
<td>1.8</td>
</tr>
<tr>
<td>NG + 10% Ethane</td>
<td>82</td>
<td>16.0</td>
<td>0.8</td>
<td>0.3</td>
<td>0.9</td>
<td>1.8</td>
<td>3.3</td>
<td>5.0</td>
<td></td>
</tr>
<tr>
<td>NG + 2% Propane</td>
<td>90.8</td>
<td>5.9</td>
<td>2.0</td>
<td>0.3</td>
<td>1.0</td>
<td>2.1</td>
<td>3.1</td>
<td>5.1</td>
<td>8.0</td>
</tr>
<tr>
<td>NG + 4% Propane</td>
<td>88.8</td>
<td>5.8</td>
<td>4.1</td>
<td>0.3</td>
<td>1.0</td>
<td>1.9</td>
<td>3.0</td>
<td>4.8</td>
<td>7.3</td>
</tr>
<tr>
<td>NG + 8% Propane</td>
<td>85.1</td>
<td>5.8</td>
<td>7.8</td>
<td>0.3</td>
<td>1.0</td>
<td>2.0</td>
<td>2.8</td>
<td>3.4</td>
<td>4.8</td>
</tr>
<tr>
<td>NG + 1% Butane</td>
<td>91.2</td>
<td>5.9</td>
<td>0.9</td>
<td>1.0</td>
<td>1.0</td>
<td>1.8</td>
<td>2.6</td>
<td>4.4</td>
<td>5.2</td>
</tr>
<tr>
<td>NG + 1.6% Butane</td>
<td>90.7</td>
<td>5.8</td>
<td>0.9</td>
<td>1.6</td>
<td>1.0</td>
<td>2.1</td>
<td>3.3</td>
<td>4.9</td>
<td></td>
</tr>
<tr>
<td>NG + 2.8% Butane</td>
<td>89.5</td>
<td>5.8</td>
<td>0.9</td>
<td>2.8</td>
<td>1.0</td>
<td>2.3</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NG + 4.2% Ethylene</td>
<td>87.6</td>
<td>5.8</td>
<td>0.9</td>
<td>0.3</td>
<td>4.2</td>
<td>1.8</td>
<td>2.4</td>
<td>3.2</td>
<td>5.2</td>
</tr>
<tr>
<td>NG + 8.5% Ethylene</td>
<td>83.9</td>
<td>5.4</td>
<td>0.9</td>
<td>0.3</td>
<td>8.5</td>
<td>1.0</td>
<td>1.6</td>
<td>2.0</td>
<td>3.1</td>
</tr>
<tr>
<td>NG +16% Ethylene</td>
<td>76.8</td>
<td>5.2</td>
<td>0.8</td>
<td>0.3</td>
<td>16.0</td>
<td>0.9</td>
<td>0.9</td>
<td>1.5</td>
<td>2.9</td>
</tr>
<tr>
<td>NG + 4% Hydrogen</td>
<td>87.9</td>
<td>5.8</td>
<td>0.9</td>
<td>0.4</td>
<td>4.0</td>
<td>1.0</td>
<td>2.3</td>
<td>2.9</td>
<td>3.7</td>
</tr>
<tr>
<td>NG + 8% Hydrogen</td>
<td>84</td>
<td>5.5</td>
<td>0.9</td>
<td>0.4</td>
<td>8.2</td>
<td>1.0</td>
<td>2.0</td>
<td>2.1</td>
<td>3.8</td>
</tr>
<tr>
<td>NG +16% Hydrogen</td>
<td>76.7</td>
<td>4.9</td>
<td>0.8</td>
<td>0.3</td>
<td>16.4</td>
<td>0.9</td>
<td>1.9</td>
<td>2.3</td>
<td>4.6</td>
</tr>
<tr>
<td>NG + 53% CO2</td>
<td>43</td>
<td>2.9</td>
<td>0.5</td>
<td>0.2</td>
<td>0.5</td>
<td>0.5</td>
<td>10.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NG + 31% CO2</td>
<td>63.4</td>
<td>4.1</td>
<td>0.6</td>
<td>0.3</td>
<td>0.7</td>
<td>31</td>
<td>7.2</td>
<td>&gt;10</td>
<td></td>
</tr>
<tr>
<td>NG + 12.5% CO2</td>
<td>79.8</td>
<td>5.6</td>
<td>0.8</td>
<td>0.3</td>
<td>0.9</td>
<td>12.6</td>
<td>3.0</td>
<td>4.7</td>
<td>7.1</td>
</tr>
</tbody>
</table>

(Note: the shaded area indicates the operating limit given by an ignition delay of approximately 3 ms.)
Agarwal and Assanis [1997] reported different results in their modeling work of the effect of natural gas composition on ignition delay using the DRM 22 code, but they claimed that the experimental results observed by Naber et al. in the constant volume combustion bomb had the same trend as their solution. Their conclusion was that “At lower temperatures, the effect of composition on delay is not distinguishable in the coordinates of the plot. The composition probably does not play a significant role at lower temperature, but becomes important at higher temperature.” Their simulation results are presented in figure 1.8. From this figure, it can be seen that although composition was claimed to play an important role on ignition delay at higher temperature, the differences were still trivial, e.g., at 1250 K, the ignition delay difference between the pure methane and high ethane content natural gas was less than 0.1 ms, and at 1600 K, the difference was less than 0.003 ms.

Figure 1.8 Variation of ignition delay for different fuels. The ambient density is 20.4 kg/m$^3$ for each case [Agarwal and Assanis, 1997].
The conclusion by Aesoy was more reasonable and achieved greater acceptance as discussed in following paragraph. Natural gas composition has a significant effect on ignition delay time at lower glow plug temperatures and has less effect at higher temperatures. This temperature effect is the opposite found by Agarwal and Assanis. But from both of their results, they all agreed that with higher alkane additives, the trend is to reduce ignition delay time.

The reason for their contradiction in temperature effect may be that their experimental setups were different: Aesoy used a glow plug in a combustion bomb, and evaluated ignition as a function of the temperature of the hot glow plug, while the temperature of the charge air was kept the same, around room temperature. Agarwal did not utilize a hot surface for ignition assistance; ignition was evaluated as a function of the hot charge air temperature.

Although higher alkane additives can reduce the ignition delay time, they also bring disadvantages to combustion emissions: higher alkane additives may increase soot emissions compared to pure methane because the carbon-carbon bonds in their molecular structure can lead directly to the formation of soot precursors; higher alkane additives may also increase the NO\textsubscript{x} formation rate due to the higher adiabatic flame temperature for the combustion of higher alkane fuels.

1.4.3 Charge Air Pressure

With a higher charge air pressure, the ignition delay will decrease, due to a higher concentration of air molecules and combustion radicals available for the same amount of fuel injection, then the chemical reaction speed will be faster. This is also implied by the Arrhenius form (equation 1.1) [Willi and Richards, 1994].
Figure 1.9 shows the experimental result of the charge air pressure effect on ignition delay by Aesoy and Valland [1996]. Figure 1.10 shows the modeling result of same effect by Agarwal and Assanis [1997]. They all suggested the same trend of the charge air pressure effect on ignition delay. This effect is important especially for a heavy duty supercharged engine due to much higher cylinder pressure.

Figure 1.9 Ignition delay as a function of charge air pressure (compression pressure) [Aesoy and Valland, 1996].
Figure 1.10 Variation of chamber pressure with time for three different ambient densities for natural gas fuel at initial temperature of 1100K [Agarwal and Assanis, 1997]. Note: The time when the pressure rises corresponds to the ignition delay time.

The experimental results by Fraser [1988] concluded that as air pressure in the combustion bomb increased, the auto ignition delay was not decreased as expected. This might be because of the unique technique he used to achieve higher temperature to simulate the end of compression condition of a real engine. A pre-designed mixture of N₂, O₂, and H₂ was ignited to have the ignition products similar with the components and concentration to fresh air, while reaching higher temperatures. This pre-ignition process might have generated some important chemical radicals that would already be present in the air at the time of fuel injection. The presence of the radicals might eliminate the effect of higher charging pressure on the ignition delay, which provides radicals with higher pressure. The experimental setup of the combustion bomb Fraser used is shown in figure 1.11.
1.4.4 Injection Conditions and Hot Surface Orientation

Injection condition includes injector nozzle numbers, nozzle hole diameter, injection direction, and injection pressure; all of these will determine the status of the injection flow. Hot surface orientation includes the hot surface shape, dimension, position, and orientation.

The injection condition together with the hot surface orientation will determine fluid flow patterns around the hot surface. This directly affects the fuel-air turbulent mixing, the heat transfer rate, and thus the ignition delay time of the fuel air mixture.

From the above summary, the injection condition and the hot surface orientation affect ignition delay time. These factors depend on the specific combustion system details. Currently it is very hard to predict and optimize these factors theoretically; optimization has, at present, to be done experimentally. But the following general trends can be stated:
1) Surface area has little influence on ignition delay time, but a great influence on ignition stability. Ignition stability is important to ensure reproducibility of cycling pressures, and it is often evaluated by the standard deviation of the maximum pressure in the cylinder. A small surface area requires a higher temperature to secure stable ignition than a larger surface area [Aesoy and Valland, 1996].

2) There is an optimum natural gas injection pressure for the shortest ignition delay. The higher the injection pressure is, the higher the momentum of the gas jet is, because the injection gas is denser at higher injection pressures. Higher momentum makes the jet velocity decay slower and jet penetration longer, so when reaching the hot surface, the gas velocity is higher. Denser gas with higher velocity passing over the hot surface makes the temperature of the hot surface lower and the residence time of the mixture around the hot surface shorter, thus increases ignition delay. On the other hand, too low an injection pressure makes the time to reach the hot surface longer and makes the mixture leaner, which will cause the penetration delay time longer and less mixture molecules around the hot surface, thus increase ignition delay time. This effect can be clearly seen from figure 1.12 [Aesoy and Valland, 1996].
3) It takes time for the hot surface to transfer its thermal energy to the surrounding mixture. Addition of a shield around or upstream of the glow plug has been proven to improve ignition delay [Aesoy and Valland, 1996; Fukuda et al., 1993]. As with glow plug conditions, the shield shape, dimensions, position, orientation, and perforations will determine the flow patterns around the glow plug affecting ignition delay time. Figures 1.13 and 1.14 show the effects of the glow plug and shield on the ignition delay measured by Aesoy and Valland [1996] in a constant volume bomb, and by Fukuta et al. [1993] in a direct injection engine, respectively.
Figure 1.13 Ignition qualities of different surface geometries as a function of temperature [Aesoy and Valland, 1996]

Figure 1.14 Two optimum shapes of glow plug shield out of 4 tested shapes. Type A shield achieved best performance of ignition assist at full load; Type B at half load [Fukuda et al., 1993].

The present chapter has summarized experimental research on the DING engines. The next chapter of the thesis will describe the complementary simulation research in the literature and then will set out the objectives for the research of this thesis.
Chapter 2

Simulation Research Background and Thesis Objectives

Simulation is an important tool for engine research work. It not only helps to understand the physics for the processes, but also provides the means for predicting performance that can be used in hardware development optimization, saving cost and time compared to experimental optimization. Much simulation work has been conducted on DING engines [Tang, 1997; Sun, 1999; Ouellette et al., 1998; Ouellette and Hill, 2002; Johnson, 1995; Li et al., 2005; Papageorgakis et al., 1996; Agarwal and Assanis, 1997].

However, there are two areas that have not been adequately covered by these existing studies. The most fundamental problem with the studies to date is that the physics of ignition by glow plug is not well understood. Thus, the key goal of the present research is to develop a complete physical representation - a mathematical model - of the processes involved in glow plug ignition. Experimental studies conducted by Abate [2001], Fabbroni [2004], and Wager
provide a means of validating the model developed. The mathematical model can then be used to simulate DING engine performance where glow plug ignition is used.

Another limitation of previous studies is that fuel injector dynamics were not modeled. The requirements for gaseous fuel injectors have been described by Green and Wallace [1989]. Due to the low density of gaseous fuels compared to conventional liquid fuels, a larger injector is required to provide adequate mass flow rate of the fuel. A larger injector means slower actuation times. A 1 ms actuation time, which is typical for a gaseous fuel injector, is significant when compared to an ignition delay period less than 2 ms. During the injection actuation period, the natural gas flow rate is controlled by the injector pintle valve rather than the nozzle. This is in contrast to the fully open case, where the natural gas flow rate is controlled by the nozzle dimensions. The flow transition during the injector actuation period will deliver fuel lower momentum than in the fully opened condition. Lower momentum means reduced mixing with air, which will in turn influence the ignition process. Thus, the fuel injector dynamics must be included to accurately model the glow plug ignition process. The following section will describe the natural gas fuel injection and glow plug ignition processes in more detail.
2.1. Simulation Research Background

2.1.1 Simulation of Gas Injection

The natural gas injector is one of the two technical difficulties for DING engine technology. Developing a reliable high pressure natural gas injector, which can consistently inject accurate amount of fuel within a short time, is an important task for the DING engine. Figure 2.1 shows the schematic of the natural gas fuel injector used in Engine Research and Development Laboratory (ERDL), University of Toronto. Originally developed by Green and Wallace [1989], figure 2.2 shows the close up view of the injector pintle, nozzle, and sac volume in the most recent version, as modified by Fabbroni [2004].

Figure 2.1 Natural gas fuel injector schematic [Fabbroni, 2004].
Sealing the injector for natural gas is much more difficult than sealing liquid diesel fuel. Metal-to-metal sealing is not suitable for a natural gas injector. Soft materials with high temperature endurance need to be researched and developed for effective sealing. Metal-to-nylon sealing was developed to achieve no leakage at 3000 psi and 444 K, as reported by Fraser [1988], but nylon creep became a significant problem and it was suggested that this be further researched.

Injection hole size, number, orientation, pintle lift, and injection duration are also very important parameters for the design of the natural gas injector. It is more difficult to ensure an energy equivalent amount of natural gas compared to liquid diesel fuel can be injected into the cylinder within the small amount of time available due to the lower density of gaseous fuel.

Modeling the internal flow in the injector is very important, because not only can the effects of injector design parameters be studied, but also the correct flow conditions at the nozzle exit can be calculated. The nozzle exit conditions are the inlet boundary conditions for the
combustion chamber and are therefore very important for further research on the injection and combustion in the combustion chamber, including interaction among the multiple jets.

Because of the complication of the injector and its internal flow, to date, no research has been published on the flow development inside the injector. Previous research on DING engine simulation used either the velocity boundary condition or the pressure boundary condition to simplify the problem of the gaseous fuel injection process into the combustion chamber.

2.1.1.1. Velocity Boundary Condition

Previous models of the natural gas injection process usually made an assumption of temporally-unchanged and spatially-uniform sonic velocity at the injector nozzle exit over the entire injection duration due to the flow choking [Tang, 1997]. Figure 2.3 illustrates the velocity boundary condition. Although this simplifies the modeling, it ignores transient details of the gas injection process and flow development inside the injector. The transient fuel jet behavior and its interaction with the glow plug strongly influence the ignition and subsequent combustion processes.

![Figure 2.3 Illustration of velocity boundary condition.](image)

To improve the velocity boundary condition, some researchers use a spatially-predetermined velocity profile with a temporally-varying velocity history, either by theoretical
analysis or from an experimental results library [Ouellette et al., 1998; Ouellette and Hill, 2002; Li et al., 2005]. This improvement considers the effects of the varying pressure difference between the injector and combustion chamber during the injection process after the combustion starts and generates a more accurate simulation result compared to the simple velocity boundary condition.

2.1.1.2. Pressure Boundary Condition

Some researchers have numerically modeled the nozzle itself by applying a constant pressure over a plane at the entrance to the nozzle or at a leading volume before the entrance of the nozzle to compute the nozzle exit velocity [Sun, 1999; Johnson et al., 1995; Papageorgakis et al., 1996]. Figure 2.4 illustrates the pressure boundary condition, which automatically considers the interaction between injector pressure and combustion bomb pressure.

![Illustration of pressure boundary condition.](image)

However, in a real injector, the pressure at the nozzle entrance is not constant over the whole period of injection because the injector pintle controls the flow during injector opening and closing. Thus, the constant pressure boundary condition is not representative of the actual injection process.
2.1.2 Simulation of Glow Plug

The flow pattern around the glow plug is affected by complicated factors such as the injecting parameters discussed above, and also by the glow plug geometry and shield orientations. The flow pattern is very important since it determines the ignition delay of the mixture.

Some modeling work has been done to simulate natural gas injection, mixing, ignition, combustion, and emissions of the glow plug assisted DING engine [Agarwal and Assanis, 1997; Papageorgakis et al., 1996], most of which used KIVA-3. Papageorgakis et al. [1996] conducted parametric studies on injector hole orientation and the number of holes. Furthermore, their study revealed the effects of the glow plug, which modified not only the temperature distribution around it, but also the flow and mixing patterns in its vicinity. However, due to the inability of KIVA-3 to perform fully 3D meshing and modeling for the complicated glow plug and shield geometry, the glow plug was modeled simply as several stepped blocks as shown in figure 2.5. This simplification limited the extent of the research situations and the computational results when compared to the real world.
Figure 2.5 Illustration of the limitation of the simple “stepped block” model to simulate glow plug [Papageorgakis et al., 1996].

Sun [1999] developed a glow plug model with a more realistic shape of a cylindrical glow plug in the combustion chamber as shown in figure 2.6. This glow plug model simulated the jet flow interaction with the glow plug, including the important gas attachment effects and residence time essential for the glow plug assisted ignition. But Sun only generated the real shape of the glow plug without a shield due to the inability of original KIVA mesh generator to account for the shield’s complex shape. For normal engine applications, the bare glow plug cannot ignite the mixture because of the short residence time and the strong cooling effect created by the cold natural gas jet impinging on it. In Sun’s glow plug model, the glow plug heat release model was simplified by assigning the temperature of the gaseous cell surrounding the glow plug the same temperature as the glow plug. This assignment will tremendously overestimate the heating effect from the glow plug. Simple theoretical calculation shows that the heat release rate predicted by this model can be as much as 14 times more than the glow plug rated
power of 100W. This over-estimation might be one of the reasons that his model computed ignition realization from a bare glow plug with short ignition delays, something not achieved in experiments.

Thus, not only should a correct glow plug and shield geometry be considered, but more importantly, a correct heat release model from the glow plug to the surrounding gas needs to be developed.

![Figure 2.6](image)

Figure 2.6   The flow pattern of the jet interacts with the glow plug from Sun’s glow plug model [Sun, 1999].

### 2.2. Objectives

This thesis will study the natural gas fuel injection process numerically, and will study the physics of the glow plug assisted natural gas ignition process by theoretical analysis based on both numerical and experimental results. The natural gas injection model will be used to investigate the natural gas ignition, combustion, and emissions. The plan is to develop the models for simulating the DING engine injection, ignition and combustion processes based on an
understanding of the physics of these processes, so as to facilitate further research on optimization of the design parameters for the gas injector, glow plug, and combustion system.

2.2.1 Modeling of the Injection from Natural Gas Injector

As discussed before, although the velocity boundary condition and the pressure boundary condition can simplify the injection process, neither of them can describe the exact transient flow characteristics at the nozzle exit. They also ignore the internal gas flow and its development within the injector, these can be very important for researching the design parameters for the natural gas injector, which is one technical difficulty for DING engine research.

The first objective for this thesis is to develop a natural gas injector model, which can model the natural gas internal flow within the injector, and research flow development inside the injector for future optimization of the injector design. It includes the effects of valve size and shape, lift, injection duration, injector sac volume, and injection pressure. With the correct injector model, effects of nozzle size, shape, numbers, and interaction between multiple jets will also be researched.

The poppet valve model in KIVA-3V can be adopted and modified for the injector model research (idea as illustrated in figure 2.7). Furthermore, a real shaped pintle model will also be developed and compared to the poppet valve model.
2.2.2 Modeling of the Ignition from the Glow Plug

Currently no proper glow plug model exists for studying ignition, which is another technical difficulty for DING engine research.

Thus, the other objective of this thesis is to study the physics of the glow plug assisted natural gas ignition process, and to develop a glow plug model, which can model this physics of the ignition phenomenon from the glow plug assistance. First, this requires setting up a model having the complicated shapes of the glow plug and its shield. Then further research can be conducted on the flow characteristics by jet interaction with the glow plug, including the gases attachment to the glow plug and the residence time of the flammable mixture surrounding the glow plug. Second, it also requires setting up a proper heat release model to understand the physics of the ignition phenomenon.

Since the very cold gas jet impinges on the glow plug at certain locations, the temperature variation on the glow plug itself cannot be neglected, which suggests that the glow plug has to be
considered in many different small elements. So this model will need to couple the gaseous region surrounding the glow plug with the solid domain of the glow plug discretized into small finite elements.

Previous research [Sun, 1999] in which the surrounding gas cells were simply assigned the same temperature as the glow plug extremely overestimates the heat release rate from the glow plug. This reveals that only a very thin layer of the surrounding gases can be effectively heated up by the glow plug. Within this thin layer, typically just micrometers, not only the heat transfer needs to be studied, but also chemical reaction and mass diffusion. These complicated physics have to be considered and all included in the glow plug model.

With the proper glow plug model, this research will study the flow pattern around the glow plug and shield, then further determine the ignition delay and flame propagation, as well as predict the combustion and emissions by investigating the factors such as shape, dimensions, positions, and orientations of the glow plug and its shield, as well as glow plug temperature, charge air temperature and pressure.

In the simulations of this thesis research work, natural gas fuel is used as pure methane for simplicity of chemical reactions in comparison to the natural gas supply in the experiments conducted at ERDL with 90% of methane mixed with other compositions, the details of which can be found in [Abate, 2002 and Fabroni, 2004].
Chapter 3

Definition of the Simulation Environment

The simulations carried out in this thesis research are part of an overall DING engine research program including both experimental and numerical work. The two components are complementary.

This chapter describes the experimental apparatus used for the simulations.

To study the natural gas injection and ignition, a constant volume combustion chamber is a suitable apparatus. Ensuring that the initial state in a combustion chamber is representative of conditions in a real engine at the time of injection is essential to the study of the natural gas injection and combustion process in the chamber [Aesoy and Valland, 1996; Agarwal and Assanis, 1997]. This constant volume combustion chamber should also have a geometry and a flow field similar to that of the engine combustion chamber.

In this research work, a CFR engine connected with a combustion chamber is utilized. The experimental apparatus used in this study has evolved over more than a decade at Engine
Research and Development Laboratory (ERDL), University of Toronto. Details of the components of the system and their operation can be found in the references [Abate, 2001; Brombacher, 1997; Cheung, 1997; Fabbroni, 2004].

3.1. Introduction to Experimental Setup

This section introduces the experimental setup that provided data for validation of the simulations in this thesis. The experimental research was conducted by a series of M.A.Sc. students [Abate, 2001; Fabbroni, 2004; Wager, 2008].

An apparatus combining a constant volume combustion chamber coupled to a single-cylinder CFR (Cooperative Fuel Research) engine through its spark plug port was developed at ERDL. The engine provides rapid compression to create realistic engine conditions (pressure and temperature) in the combustion chamber, and also scavenges combustion products. Because the clearance volume of the engine has been reduced and the total final compression ratio is adjusted to 16.51 : 1; almost all of the air in the cylinder is forced into the combustion chamber during compression. The combustion chamber volume is representative of the clearance volume of a DI passenger car diesel engine. The 3-D view and top view of the CFR engine and the connected combustion chamber are shown in figure 3.1 and figure 3.2. The tangential entry of the spark plug port from the CFR engine cylinder provides a strong swirling flow, which is typical of the flow in a diesel engine cylinder. The absence of valves, ports, and cooling passages from the combustion chamber walls allows considerable flexibility in positioning the fuel injector and glow plug. It also permits installation of a quartz window that provides optical access with a piston-side view similar to that obtained by viewing through a Bowditch piston assembly, which
is a traditional method in the engine research field to allow laser and camera access through an optical piston assembly first proposed by Bowditch [1961].

Figure 3.1 3-D View of CFR Engine with ERDL Combustion Chamber and Natural Gas Injector [Abate, 2001]

Figure 3.2 Top View of CFR Engine and ERDL Combustion Chamber Details [Abate, 2001]
The constant volume combustion chamber mimics the combustion chamber of a typical medium speed diesel engine with a bowl-in-piston design. The geometry is illustrated in figure 3.3. The tangential entry port connecting the cylinder with the combustion chamber has a diameter of 9.53 mm and a total length of 48 mm. The combustion chamber is closed by a quartz window (figure 3.2). The resulting combustion chamber has a diameter of 50.8 mm and a depth of 12.7 mm.

Figure 3.3    Tangentially Oriented Combustion Chamber Charging Passageway for Swirl Generation [Fabbroni, 2004]

A flat plate with machined valve depressions was added by researchers at ERDL to the top of the CFR engine piston to minimize the cylinder clearance volume. This produced a minimal 0.45 mm piston-to-cylinder head clearance. The three volumes, combustion chamber, tangential passage, and the cylinder clearance volume combine for a total clearance volume of
39.44 cm$^3$. This value of the total clearance volume also accounts for the volume occupied by the fuel injector nozzle and glow plug, as well as other CFR engine cylinder head cavities. With the CFR engine displaced volume of 611.7 cm$^3$ (82.55 mm bore x 114.3 mm stroke), a nominal compression ratio of 16.5:1 is achieved.

To prevent possible fouling of the combustion chamber window, a second oil control ring was added to the CFR piston in order to minimize oil entry into the combustion chamber. In operation, the CFR engine was motored between 200-400 rpm, driven by variable speed DC motor. With an operating speed of 230 rpm, the tangential entry port generates a swirling flow with an approximate swirl intensity of 3622 rpm (or 60.4 Hz, see subsequent section for details). This angular velocity is representative of current engine practice. For example, a diesel engine having a swirl ratio of 2 running at 1800 rpm would have the same in-cylinder angular velocity.

The solenoid-actuated gaseous fuel injector was originally developed by Green and Wallace [1989]. Later modifications at ERDL to the original design include a new nozzle design, a revised driver circuit and a revised lift sensor. The injector is located in the center of the chamber. The tip of the injector has a length of 12.7 mm (0.5”) projected into the chamber from the chamber top surface. Its diameter is 6.35 mm (0.25”). The injector can be altered so that the effect of different number and diameter nozzle orifices on injection processes can be examined. The injector is supplied with natural gas at 11 MPa from compressed gas cylinders. Injection is controlled by a Labview program acting through an injector driver circuit. In practice, the injector is skip fired during experiments to remove residual gases between fired cycles and to reduce the thermal load on the quartz window. For the specified clearance volume employed, skipping four cycles nominally removes 99.99% of the residual gas.
A glow plug is inserted into the combustion chamber near to the injector nozzle exit in order to ignite the fuel jet for combustion. The orientation of the injector and the glow plug in the combustion chamber is illustrated in figure 3.3. The details of the glow plug dimension and functional parameters will be introduced further in chapter 5.

Undiluted ethylene glycol is circulated through the cylinder head and block of the CFR engine to reduce heat transfer losses during the compression stroke and thereby attain higher peak temperatures in the combustion chamber. A Haake N3 bath heater/circulator can produce glycol temperatures up to 155 °C. The combustion chamber itself was wrapped by a 400 W Omegalux rope heater (FGR-080) that was used to bring the combustion chamber up to operating temperature rapidly and to maintain constant temperature with skip firing.

Air inlet temperature and pressure can be controlled independently and can be varied to achieve specific in-cylinder conditions at the time of injection. A 1000 W electric resistance heating element located in the air inlet produces intake air temperatures up to 350 °C. The air inlet is connected to a shop air supply with an adjustable pressure regulator. Intake pressures ranging from atmospheric up to a maximum of 30 psig have been used in the test program.

3.2. Experimental Results

Experiments were conducted to characterize the constant volume combustion chamber. Experimental details can be found in Abate’s and Fabbroni’s work [Abate, 2001; Fabbroni, 2004].

Using the typical motored pressure and temperature profiles measured in the constant volume combustion chamber and the ideal gas equation of state, the transient mass contained in
the constant volume combustion chamber can be calculated. Thus, the average air velocity entering through the connecting port from cylinder to the combustion chamber can be calculated from the mass change in the combustion chamber. The maximum average velocity entering is only about 30 m/s due to the large connecting port diameter (9.53 mm). The delay of the pressure difference between the constant volume combustion chamber and the engine cylinder is negligible, as confirmed from simultaneous measurements from pressure transducers placed in the cylinder (on the cylinder head) and in the constant volume combustion chamber [Fabbroni, 2004].

Swirl intensity is a very important parameter affecting ignition, combustion, and flame propagation. In the absence of direct velocity measurements, swirl was estimated [Abate, 2001]. Figure 3.4 shows combustion images taken using an intensified CCD (ICCD) imaging system and shows the soot cloud (black area) propagation for an ignited gas jet in the swirling air in the combustion chamber. The soot cloud allows a form of particle tracking. By measuring the movement of the leading edge of the soot cloud, the swirl angular velocity can be estimated. The images shown in figure 3.4 were used to determine the swirl angular velocity at a motored engine speed of 200 rpm. The average swirl intensity concluded from the images was about 380 rad/sec, or 3622 rpm (60.4 Hz).

Figure 3.4 Combustion images used for determining swirl angular velocity (negative image used for clarity, and time intervals are shown from the start of injection point) [Abate, 2001].
The timing shown in figure 3.4 can be translated into crank angle as 7-13 crank angle degree (CAD) after top dead center (ATDC), with an average of 10 CAD ATDC. Since the time intervals were shown from the start of injection, which was 11 CAD before top dead center (BTDC), with the engine running at 200 rpm, 15 ~ 20 ms corresponding to 7 ~ 13 CAD ATDC, of which the median is 10 CAD ATDC.

3.3. Simulation of Swirl Formation

A numerical model of the CFR engine and the combustion chamber with their connecting passage was set up using the exact dimensions of the experimental apparatus in order to study the initial state of pressure and temperature distribution in the combustion chamber and to characterize the swirl velocity profile.

Swirl is a very important parameter affecting ignition, combustion, and flame propagation. However, we lack detailed experimental results of the swirl intensity and profile due to the difficulty of direct air velocity measurements in an engine application, e.g., the conventional hot wire method is difficult to apply in terms of mounting in a high temperature combustion environment. Thus, a numerical simulation was conducted to determine the time-varying swirl characteristics. The determined swirl velocity profile will be imposed onto a simplified enclosed domain consisting of only the combustion chamber itself, so that a much denser mesh structure could be used for future research in injection and ignition in the combustion chamber for improving computation accuracy.

Some modifications of the KIVA mesh generator were made to accommodate the special shape of the mesh, such as the generation of a cylinder in the z-axis for the combustion chamber (see the list of code modifications in appendix A.1). Figure 3.5 presents the numerical research
domain and the mesh structure (a grid convergency study is introduced in section 3.5) and it clearly shows the tangential entry port mentioned earlier but not visible in figure 3.1.

![3-D view of research domain and the side view of the cross section of the mesh structure.](image)

Figure 3.5. 3-D view of research domain and the side view of the cross section of the mesh structure.

The computation was started at the beginning of the compression stroke at bottom dead center (BDC) of piston position with initial conditions of 400 K temperature, 101 kPa pressure, 400 K wall temperatures, and 200 rpm engine speed, to match the experimental data from Abate [Abate. 2001]. The computation was ended at the end of the expansion stroke (BDC), which simulated 360 crank angle degree (CAD).

The simulation results of the combustion chamber pressure and temperature are shown in figure 3.6. It reveals that although the peak temperature in the combustion chamber is lower than
the one in the cylinder, the combustion chamber pressure is nearly the same as the cylinder pressure in good agreement with the experimental results.

![Graph showing computed in-cylinder and combustion chamber pressure and temperature.](image)

**Figure 3.6**  Computed in-cylinder and combustion chamber pressure and temperature.

The swirl intensity in the combustion chamber reached the maximum of 680 rad/sec (6494 rpm or 107.8 Hz) for the swirl angular velocity at about 20 CAD BTDC. Swirl is not solid body rotation: it has different angular velocities at different radii. To match with the experimental results which were measured at near wall position shown in figure 3.4, the swirl angular velocity in figure 3.7 is defined as the angular velocity at near wall position.

The swirl is generated by piston motion. Figure 3.7 shows a maximum upward piston velocity ratio of 1.68. With an average mean piston speed $S_{p\text{ average}} = 0.762$ m/s, this corresponds to a piston velocity of 1.28 m/s at about 70 CAD BTDC. The piston velocity remains above 0.5 m/s until 20 CAD BTDC. A piston velocity of 0.5 m/s produces an air flow velocity through the connecting port of more than 35 m/s, calculated using a simple ratio of port cross-sectional area to piston area. At top dead center, the swirl intensity decreased to 484 rad/sec (4621 rpm or 77.0
Hz). At 9.8 CAD ATDC of piston position, the swirl intensity dropped to 380 rad/sec (3622).

This showed satisfactory agreement with the experimental results.

Figure 3.7    Computed swirl intensity and piston velocity vs. crank angle.

3.4.   Swirl Intensity and Profile Determinations at Top Dead Center

A typical computed velocity field in the combustion chamber at engine top dead center
(TDC) is shown in figure 3.8.

Figure 3.8    Representative computed velocity field at TDC.
The swirl profile computed using the model embedded in the KIVA-3V code, uses a Bessel function with recommended parameters, is shown in figure 3.9. The peak swirl location is at about the 2/3 radius position. This profile is suitable for most engine applications since the swirl is generated by the induced air during the intake process, and it also shows the effects of the cylinder wall friction. However, the embedded profile may not be suitable for the present combustion chamber because the fundamentals of swirl formation are different.

![Swirl profile along the radial direction.](image)

Figure 3.9 Swirl profile along the radial direction.

The simulation results show that the swirl profile has a maximum value near the combustion chamber wall position (figure 3.9), because air is compressed into the combustion chamber during the compression process tangentially near the outside of the combustion chamber wall.

Thus, original parameters recommended by KIVA in the Bessel function had to be modified to describe the special swirl profile in the ERDL combustion bomb chamber according to the simulation result. The final adjusted swirl profile is shown in figure 3.9, and this profile
was used in all subsequent simulations of glow plug ignition. The detailed modification for Bessel function is introduced in Appendix B.

3.5. Independence Study of Mesh Density

The sensitivity of velocity results to mesh selection was studied using the three meshes described in Table 3.1.

<table>
<thead>
<tr>
<th>Case</th>
<th>Cylinder</th>
<th>Bomb</th>
<th>Total cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse mesh</td>
<td>23×28×30</td>
<td>5×6×5</td>
<td>19605</td>
</tr>
<tr>
<td>Regular mesh</td>
<td>28×28×30</td>
<td>7×8×6</td>
<td>27293</td>
</tr>
<tr>
<td>Fine mesh</td>
<td>28×44×30</td>
<td>10×10×8</td>
<td>42677</td>
</tr>
</tbody>
</table>

Figure 3.10 shows the mesh dependence study on three cases: course mesh, regular mesh, which is the described mesh above, and fine mesh. As the density of the grid in the combustion bomb is increased, the number of cells in the engine cylinder increase dramatically due to the need to patch the cells to match the combustion bomb grid in the passageway. The results in figure 3.10 show that the average difference between the regular and fine meshes was 5.7%. As grid selection is a compromise between accuracy and computational time, the regular grid structure was deemed to produce adequate results and was used for the calculations presented in figure 3.10.
3.6. Initial Condition Setup for Combustion Chamber

After having characterized the swirl velocity in the combustion chamber, further numerical research into the injection and combustion processes in the combustion chamber need only consider the combustion chamber itself as the research domain without the engine cylinder and connecting passage. This will simplify the mesh structure and increase the mesh density so as to increase the accuracy of the computation. Figure 3.11 illustrates the simplified combustion chamber configuration that will be used in future computations.
As a summary, the initial condition for future simulation of the combustion chamber is listed in Table 3.2. To match the experimental conditions conducted at ERDL, the temperature and pressure at TDC were chosen the same as the experiments rather than the simulation results, although they have good agreement with each other.

Table 3.2. The list of initial conditions for the simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion chamber pressure</td>
<td>4 MPa</td>
</tr>
<tr>
<td>Combustion chamber temperature</td>
<td>850 K</td>
</tr>
<tr>
<td>Wall temperature</td>
<td>400 K</td>
</tr>
<tr>
<td>Swirl Intensity</td>
<td>Adjusted swirl intensity profile as in figure 3.9</td>
</tr>
<tr>
<td>Injection pressure</td>
<td>11 MPa</td>
</tr>
<tr>
<td>Injection temperature</td>
<td>400 K</td>
</tr>
</tbody>
</table>
Simulation of the swirl effect on the jet was conducted after setting up the new domain and using the poppet valve model for the methane injection. This poppet valve model will be introduced in chapter 4. The initial conditions used for this simulation is the same as listed in 3.2, the nozzle diameter is 0.5 mm. The swirl simulation result is as shown in figure 3.12, where the tracking parameter is chosen to be stoichiometric mixture outline (fuel air equivalence ratio of 1).

![Swirl Effect Diagram](image)

Figure 3.12 The computed swirl effect on the jet in combustion chamber.

Noted that there may be other possible methods for tracking the swirl intensity such as using centroid displacement of the jet instead of the downstream leading edge of jet at fuel air equivalent ratio of 1 profile. However, for the method of tracking centroid displacement of the
jet, there might be radial movement besides the rotational movement (thita direction), which makes comparison relationship more complex. The chosen method of tracking the downstream leading edge of jet at fuel air equivalent ratio of 1 profile for swirl intensity simulation is much convenient and similar compared to the experimental approach, which used downstream leading edge of the soot images.

The swirl intensity from the simulation is 4050 rpm (or 67.5 Hz), which is about 12% smaller than the initial swirl intensity of 4621 rpm (or 77 Hz). The combustion chamber wall friction from the swirling flow may play a role in this decrease, and also the inertia of the cold denser jet compared to swirling air environment will make the jet swirling speed a little smaller than the initial swirling air speed.

However, compared to the experimental results of swirl visualization in figure 3.4, this simulation qualitatively agrees well with the experiments, taking into consideration the lack of detailed initial conditions of the experiments as well as the different tracking factors used, i.e., the soot cloud in the experiments vs. the fuel-air equivalence ratio in the simulation. Besides these differences, the experimental images of the soot cloud in figure 3.4 shows the integrated images drawing from the optical edge of a variety of the planes in the whole 3-D bomb space, while as comparison, the simulation pictures in figure 3.12 only show a slice at the central plane of the jet, thus they are not direct comparable to each other.

### 3.7. Conclusions

Numerical simulation confirms the experimental results that the delay and difference of the in-cylinder pressure and combustion chamber pressure were negligible, and air velocity in the connecting port lower than 35 m/s.
The calculated swirl angular velocities were 484 rad/sec (4621 rpm or 77.0 Hz) at TDC and 380.3 rad/sec (3622 rpm or 60.4 Hz) at 9.8 CAD ATDC, which showed satisfactory agreement with the experimental results.

The angular velocity profile calculated for the combustion chamber is different from the one calculated from the original parameters recommended by KIVA in the embedded Bessel function. The parameters in the Bessel function were modified to generate a suitable swirl profile according to the simulation result to facilitate future simulation of experimental results obtained using the constant volume combustion chamber.
Chapter 4

Simulation of Natural Gas Injection

The flow of natural gas from the fuel injector outlet is the inlet boundary condition for the simulation of the glow plug ignition process. It must be accurately represented in order for the subsequent ignition simulation to be accurate. As noted in chapter 2, the transient development of the natural gas flow must be accounted for.

The previous injection models based on a velocity boundary condition or a pressure boundary condition described in chapter 2 have a number of the drawbacks. Not only is inaccuracy created by assigning the velocity or pressure condition at the boundary for simplification, but also by negligence of the internal flow development within the injector. To overcome these drawbacks, a poppet valve model was proposed and developed by making use of the KIVA-3V valve model with modifications.

The KIVA-3V CFD code was developed at Los Alamos National Laboratory [Amsden, 1993; Amsden, 1999] with the source code provided as part of the purchased software. Among
its features is the ability of modeling multi-dimensional fluid dynamics, valves, fuel sprays and chemical reactions. Although the KIVA mesh generator has some restrictions and is incapable of generating a complicated geometric mesh since KIVA was designed specifically for internal combustion engine applications, its capacity for CFD computation with chemical reaction functions facilitate the next phase of the work coupling methane injection with glow plug assisted ignition and combustion processes. Thus the KIVA-3V CFD code was chosen to simulate fluid flow with some modifications made to the grid generator so as to accommodate a more general geometry.

4.1 Poppet Valve Model and Performance of Single Jet Injection

Simulation with the poppet valve model was performed to model the injector pintle lift. The pintle controls the flow of fuel gas into the injector sac volume and the resulting pressure build up in the sac volume drives fuel gas expansion through the nozzle(s) and into the combustion chamber. Although the shape of the poppet valve is not the same as the real injector pintle, the valve model works well in a fundamental study of the transient injection process within the injector. This model computes the development of velocity profile for gaseous fuel at the exit of the nozzle.

Because KIVA was not specifically designed to work for high speed gaseous flows, a problem was found that when the KIVA code deals with a pressure boundary condition for a high speed gaseous flow, it will cause a total energy increase along the streamline, i.e., at the entrance of the pressure boundary, the gas can have high kinetic energy (Mach number of 0.6) but with the same temperature as the high pressure reservoir. In an isentropic expansion, the temperature normally drops. Thus, in KIVA the total energy was over-estimated. To overcome
this problem, an isentropic relationship was applied over the entrance of the high-pressure boundary plane, so that the proper relationship between velocity and temperature, constrained by the conservation of total energy, was maintained. A detailed discussion of this modification can be found in Appendix C.

When natural gas is injected from the injector at a high pressure to the combustion chamber at a low pressure, the flow is choked at the nozzle exit. This under-expanded flow thus generates a series of shock waves downstream near to the nozzle exit. The location of the shock waves is very close to the nozzle exit (within 2-3 mm of the nozzle exit), and the glow plug is relatively far (7 mm) away from the nozzle exit. Figure 4.1 shows the location of the shock wave zone using KIVA simulation with a high density mesh when methane is injected from 11MPa to 80 kPa at 297 K through a 0.344 mm diameter nozzle.

A comparison of results with different mesh sizes (Appendix D) shows that the shock waves do not have noticeable effects on the flow pattern 7.0 mm downstream from the nozzle exit, which is the region for ignition and combustion from the glow plug. To avoid the high-density mesh for studying the shock wave phenomenon, the designed mesh is kept relatively coarse in order to have an affordable computational load for researching only the natural gas flow pattern and the further ignition and combustion in the combustion chamber. However, the study on the shock waves itself is introduced in Appendix D.
4.1.1. Poppet Valve Model

A 3D 360-degree full cylindrical mesh was generated for KIVA with newly added (by this author) function of uneven mesh generation, as shown in figure 4.2. Compared with a partial sector (e.g., 60°), a full 360° of combustion chamber generates more grid cells and requires more computational time and storage. On the other hand, the full cylinder domain not only eliminates the periodic boundary condition for a partial sector grid, which does not match the real case in the valve model, but it also facilitates the future addition of more injection nozzles to the injector mesh without too much change to the mesh structure.

Use of an uneven mesh technique significantly reduces the computational time and storage space, while refining the computational precision where needed. Several subroutines were modified and several new subroutines added to achieve the uneven mesh in all of the 3 directions. The detailed modifications are listed in Appendix A.1. As figure 4.2 shows, the nearer to the injector and nozzle, the finer the mesh is.

Figure 4.2 Illustration of mesh structure (top view and partial side view) for a three hole nozzle.
In the computation, the nozzle diameter is chosen as 0.34 mm (small nozzle) or 0.5 mm (big nozzle), the initial air temperature and pressure in the combustion chamber are 850 K and 40 bar respectively, and the methane supply temperature and pressure are 400 K and 110 bar respectively. The injector pintle lift is 0.4 mm, and the overall injection duration is 9.8 ms, chosen to be higher than normal 2~5 ms injection duration in our experiments for reasons to be described in the next section. The valve opening period is 0.005 ms, while the valve closing period is 0.8 ms, based on the experimental valve lift data.

4.1.2. Performance of Single Jet Injection

In this section, the performance of a single jet injection from the poppet valve injector model is studied, including the temperature profile and fuel air equivalence ratio profile for the single jet, and the transient internal flow development within the fuel injector.

4.1.2.1. Temperature Profile and Fuel Air Equivalence Ratio Profile

Figure 4.3 shows the computational results for the profiles of temperature and fuel air equivalence ratio ($\phi$) at 8.017 ms after injection. From the figure, it can be seen that the core temperature of the methane jet is cold (below 360 K) due to the isentropic expansion. This low temperature makes methane auto ignition difficult. The profile of the fuel air equivalence ratio shows that the main region of the jet is very difficult to mix with air. There is only a very thin outside layer surrounding the jet in which air is entrained to make a flammable zone. From the above two points and the chemical kinetics, compared with liquid fuels, natural gas is in fact more difficult to auto ignite, thus ignition assistance is required.
Figure 4.3 also shows that after the jet reaches the wall of the combustion chamber, it is reflected by the wall and moves back into the chamber.

![Figure 4.3](image)

The profiles of temperature and fuel air equivalence ratio ($\phi$) at 8.017 ms after injection.

4.1.2.1. Transient Internal Flow Development within the Injector

The velocity and Mach number comparison between 0.5 ms, 2.0 ms, and 8.0 ms after injection are shown in figure 4.4. From this figure, we can conclude that at 0.5 ms after injection, the velocity has already choked at center line of the nozzle exit at 489.7 m/s. The corresponding choking temperature is 380 K. At both 2.0 ms and 8.5 ms after injection the velocity is choked at the exit of the nozzle at 476.7 m/s, with a corresponding temperature of 351 K. The identical profiles of 2.0 ms and 8.0 ms illustrate that the flow has been fully developed, so after 2.0 ms of injection, the velocity and pressure profile will not change until ignition occurs. This is also the reason why a longer valve opening time was chosen for this research since more data from the simulation result are available for different valve shut off times. Comparing results for the 0.5 ms and 2.0 ms injection durations, the Mach number profile at 0.5 ms is nearly the same as that at

* If printed in black and white, note that the injector sac volume temperature is low, and the background of combustion chamber temperature is high on the color scale; similarly there is only pure methane in the injector sac volume and in combustion chamber background it is pure air. It also applies to the other color scale figures in this thesis.
2.0 ms, which means the velocity profile is already fully developed. However, the temperature will still be different as the change from 380 K to 351 K causes a change in velocity from 489.7 m/s to 476.7 m/s, although both velocities correspond nearly to the choking velocity at Mach number of about 1. So, the development of the temperature in the injector is slower than the development of velocity.

Figure 4.4 The velocity and Mach number comparison between 0.5 ms, 2.0 ms, and 8.0 ms after injection.

Figure 4.5-a) shows the single-humped profile for the velocity at the nozzle exit due to the effect of the nozzle wall. The mesh density for the nozzle is 4x4. A denser mesh of 8x8 for the injector was used and the same simple humped velocity profile was found as shown in figure 4.5-b). This result does not agree with either the normal assumed uniform choking velocity profile or the double-humped velocity profile simulated by Papageorgakis et al. [1996] from a pressure boundary condition using their own CFD code, but is more realistic than either.
Figure 4.5  The simulation velocity profile at nozzle exit plane.

Figure 4.6 shows the transient gas injection flow development process in the injector for pressure, velocity and temperature at the nozzle entrance and exit. From the figure, it shows that it takes about 0.8 ms for the flow to be fully developed. Within this period, pressure, temperature and velocity oscillate, and then become stabilized. The oscillation magnitude of the temperature is higher than that of the pressure. This is consistent with the previous point that pressure is stabilized faster than temperature. From the velocity transient change, it can be seen that from the start of the valve opening to the fully developed flow time, the exit velocity at the center line of the nozzle has about an 11% difference, so the assumption of the uniform velocity over the whole injection period is not very accurate.
4.2 Validation of Poppet Valve Model

4.2.1. Mass Flow Rate

The measured injector mass flow rates can be compared with the calculated theoretical values. With the assumption of 1-D isentropic flow at the nozzle exit, the theoretical mass flow rate from the injector can be deceived by the relationship of isentropic expansion [Liepmann and Roshko, 1957]:

$$ m = \frac{A_n P_0}{(RT_0)^{\frac{5}{2}}} \left( \frac{P}{P_0} \right)^{\frac{1}{\gamma}} \left\{ 2\gamma \left[ 1 - \left( \frac{P}{P_0} \right)^{\frac{\gamma - 1}{\gamma}} \right] \right\}^{\frac{1}{2}} $$

Equation (4-1)

where $A_n$ is the nozzle orifice area, $P_0$ and $T_0$ are the upstream gas pressure and temperature, $R$ is the gas constant of the injected gas, and $?^{\gamma}$ is the specific heat ratio of the injected gas. For choked flow, the pressure ratio in equation 4-1 is given by equation 4-2.
\[
\frac{P}{P_0} = \left[ \frac{2}{\gamma + 1} \right]^{\frac{\gamma}{\gamma - 1}} \quad \text{Equation (4-2)}
\]

By substituting the choking condition of equation (4-2) into equation (4-1), the mass flow rate at choking is:

\[
\dot{m} = \frac{A_n P_0}{(RT_0)\frac{1}{\gamma}} \left( \frac{2}{\gamma + 1} \right)^{\frac{1}{\gamma - 1}} \left( \frac{2\gamma}{\gamma + 1} \right)^{\frac{1}{2}} \quad \text{Equation (4-3)}
\]

Using the above equations and the known nozzle cross-section area, one can calculate the expected injection mass flow rate.

Experimental data were available for mass flow rate validation from the experiments conducted by Fabbroni [2004]. Natural gas was injected through the injector nozzle (0.344 mm diameter) from an 11 MPa supply to an average 80 kPa combustion chamber environment. The results are shown in figure 4.7. The simple 1-D theoretical analysis based on a choking condition (equation 4-3) suggested a mass flow rate of 1.76 mg/s, agreeing well with experimental data of 1.79 mg/s.
The computational result using KIVA-3V at the same condition shows that at the steady state of the injection, the mass flow rate is 1.69 mg/s. It agrees well to both of the analytical result and experimental result as shown in table 4.1.

Table 4.1 Comparison of the simulation mass flow rate to the analytical and experimental results (0.344mm nozzle, 11 MPa to 80 kPa).

<table>
<thead>
<tr>
<th>Case</th>
<th>Simulation</th>
<th>Experimental</th>
<th>Analytical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate</td>
<td>1.69 g/s</td>
<td>1.79 g/s</td>
<td>1.76 g/s</td>
</tr>
<tr>
<td>Difference</td>
<td>4.0%</td>
<td>1.7%</td>
<td>--</td>
</tr>
</tbody>
</table>

Other simulations were conducted for two sizes of the nozzles at Fabbron’s experimental conditions for the combustion chamber: an upstream pressure of 11 MPa, an upstream temperature of 400 K, a combustion chamber pressure of 4 MPa for methane to be injected into,
and a combustion chamber temperature of 850 K. The comparison of the simulation results to the analytical results calculated from equation (4-3) is shown in table 4.2.

Table 4.2 Comparison of the simulation mass flow rate to the analytical ones (11 MPa to 4 MPa).

<table>
<thead>
<tr>
<th>Case</th>
<th>Nozzle Diameter (mm)</th>
<th>Mass Flow Rate</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Simulation</td>
<td>Analytical</td>
</tr>
<tr>
<td>1</td>
<td>0.5</td>
<td>3.28 g/s</td>
<td>3.22 g/s</td>
</tr>
<tr>
<td>2</td>
<td>0.344</td>
<td>1.50 g/s</td>
<td>1.76 g/s</td>
</tr>
</tbody>
</table>

For case 2, the Mach number at the exit of the nozzle calculated by the simulation is only 0.85 instead of 1, implying that the friction for this size of the nozzle restricts the flow and prevents it from developing to the sonic flow choking at the exit because of a smaller nozzle diameter and a larger ratio of L/D (approximately 4.6). Compared to Fabbroni’s experiments, the difference is in the downstream pressure. For Fabbroni’s experiments, the downstream pressure is vacuum (80 KPa) instead of 4 MPa. This low pressure makes the pressure difference high enough to overcome the friction along the nozzle and keep on accelerating the flow until it is choking at the exit.

From comparison of the experimental and analytical mass flow rate results, the simulation has good agreement with experimental and analytical results.
4.2.2. Jet Penetration

From their experimental data on jet penetration, Ouellette and Hill [2002] proposed a dimensionless formula as equation 4-4.

\[
\frac{Z_t}{(M_n/\rho_o)^{1/4}t^{1/2}} = \Gamma
\]

where \(Z_t\) is the jet penetration, \(M_n\) is the momentum injection rate at the nozzle exit, \(\rho_o\) is the density in the chamber, \(t\) is the time from the beginning of injection, and \(\Gamma\) a constant for the turbulent jet issued from the nozzle. \(\Gamma\) is also the dimensionless number obtained from their experiments.

Ouellette and Hill [2002] concluded \(\Gamma\) to be 3.0 ± 0.1. Kuo and Bracco [1982] reported their \(\Gamma\) of 2.75, and Gaillard [1984] reported his \(\Gamma\) of 2.5, in their simulation work respectively.

Inside the KIVA-3V code, there is a set of built-in turbulence k-ε equations that contain constants \(c_1\) and \(c_2\), which are allowed to be modified within a range. Different constant values were evaluated as suggested by Ouellette and Hill [2002], changing from the original KIVA values of \(c_1=1.44, c_2=1.92\), to the current values of \(c_1=1.52, c_2=1.92\). This change made the jet penetration increase 8.4%, but the mass flow rate stays the same. The derived \(\Gamma\) for the combustion chamber in this research is 2.72 for the new set of turbulence constants for both the 0.5 mm and the 0.344 mm nozzles, compared to 2.51 for the old set of turbulent constants. Figure 4.8 shows the different results.
Figure 4.8  Simulation result of jet penetration length and the constant $\Gamma$.

In previous ERDL research, Brombacher [1997] found experimentally a value for $\Gamma$ of $2.7 \pm 0.8$. The simulation results of jet penetration agree relatively well with Brombacher’s experiments.
4.3  Mesh Density Independence Study

To study mesh density independence, injection simulations using three different densities were performed: coarse mesh, regular mesh, and fine mesh.

Compared to the combustion chamber, the injector nozzle has a relatively small dimension with a fine enough mesh, most of the computational load was restricted by the mesh density in the combustion chamber. So, all 3 of these mesh structures have the same mesh density within the injector, but different densities within the combustion chamber.

Since only one nozzle was used in each case, the total 360° combustion chamber was divided into four 90° sections (sectors). Each section (sector) has an even mesh in the $\theta$ direction. However, the section containing the nozzle has a much denser mesh than the other sections. For the $r$ and $z$ directions, the uneven mesh technique was applied. The mesh structure is shown in figure 4.9.

![Mesh structure for the grid density study.](image)

Figure 4.9  Mesh structure for the grid density study.
The details of the grid densities of these 3 meshes are listed in table 4.3, and the comparison of the mass flow rate and jet penetration computed using these 3 mesh structures is shown in table 4.4.

<table>
<thead>
<tr>
<th>Mesh structure</th>
<th>Coarse mesh</th>
<th>Regular mesh</th>
<th>Fine mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sector 1</td>
<td>19×20×24</td>
<td>23×24×30</td>
<td>29×30×36</td>
</tr>
<tr>
<td>Sector 2</td>
<td>19×11×24</td>
<td>23×14×30</td>
<td>29×18×36</td>
</tr>
<tr>
<td>Sector 3</td>
<td>19×5×24</td>
<td>23×6×30</td>
<td>29×8×36</td>
</tr>
<tr>
<td>Total cells</td>
<td>34594</td>
<td>55894</td>
<td>98090</td>
</tr>
</tbody>
</table>

Table 4.4 Comparison of the different mesh structures – computed results

<table>
<thead>
<tr>
<th>Mesh structure</th>
<th>Coarse mesh</th>
<th>Regular mesh</th>
<th>Fine mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate (g/s)</td>
<td>1.44</td>
<td>1.50</td>
<td>1.52</td>
</tr>
<tr>
<td>Difference</td>
<td>5.26 %</td>
<td>1.32 %</td>
<td>--</td>
</tr>
<tr>
<td>Jet penetration Length (cm, at 0.14ms)</td>
<td>1.07</td>
<td>1.12</td>
<td>1.14</td>
</tr>
<tr>
<td>Difference</td>
<td>6.14 %</td>
<td>1.75 %</td>
<td>--</td>
</tr>
<tr>
<td>Jet penetration Length (cm, at 0.84ms)</td>
<td>2.64</td>
<td>2.89</td>
<td>3.03</td>
</tr>
<tr>
<td>Difference</td>
<td>12.87 %</td>
<td>4.62 %</td>
<td>--</td>
</tr>
</tbody>
</table>

The convergence trend is clearly shown in table 4.4. The difference of mass flow rate between the regular mesh and the fine mesh decreased from 5.26% to 1.32% compared to the one between the coarse mesh and the fine mesh. Similar to the early time jet penetration length,
decreased from 6.14% to 1.75%. The differences in jet penetration length at late time are relatively large, since the jet reaches the larger mesh size zone far away from the nozzle because of uneven mesh structure. At the early time compared to the late time, the convergence degree of the jet penetration was improved. The uneven mesh structure contributed to this improvement, since in the region close to the nozzle, the mesh is already designed to be fairly dense compared to the region far away. This will also benefit the ignition study (to be described in chapter 7), in which the glow plug was placed near to the nozzle exit, and the initial active chemical reaction region is located surrounding the glow plug.

As the regular mesh already shows good convergence, the following study of the natural gas injection was based on this structure. For future ignition and combustion with chemical reaction and new ignition models turned on, the computational load will be a bigger concern.

4.4 Study of Natural Gas Injection

The poppet valve model just described was used to study aspects of injector operation, namely the effects of nozzle size and the interaction between multiple jets, and the effects of swirl in the region surrounding the glow plug. It was also used to study the flow features in the vicinity of a shielded glow plug.

4.4.1 Effects of the Nozzle Sizes on Natural Gas Jet and Interaction of Multiple Jets

As the nozzle diameter becomes smaller than 0.5 mm, the momentum of the injected gas flow decreases, and the penetration of the jet is reduced. The flow is choked at the exit of the nozzle. For multiple nozzles of 0.5 mm diameter, the mixing is still very poor, no air is entrained into the gas in between the jets, the jets are merged together, and the flammable region is still a
very thin layer at the outline of the jets (figure 4.10-a).

Figure 4.10 The profiles of fuel air equivalence ratio (φ) and temperature for the different size nozzle multiple jets interaction. (a) Fuel air equivalence ratio profile for 0.5 mm nozzles; (b) Fuel air equivalence ratio profile for 0.15 mm nozzles; (c) Temperature profile for 0.15 mm nozzles.

As the nozzle diameter is decreased to the critical (transition between choked and un-choked flow) value of about 0.34 mm, the ratio of L/D is about 4.6, the wall friction effects dominate in the nozzle, and the flow becomes subsonic* (Figure 4.11). As the nozzle diameter is reduced to 0.15 mm, the centerline exit velocity decreases to 243 m/s (Mach number 0.41), the penetration is also further reduced, and the mass flow rate is only 1/20 of that at 0.5 mm diameter. However, the mixing becomes better, lots of air is entrained in between the jets, and the flammable region is improved significantly (figure 4.10-b). At the same time, the temperature at the core of the jet is only reduced to about 509 K compared to the core temperature of 351 K for the 0.5 mm nozzle due to the reduced expansion and relatively more friction (figure 4.10-c). Although the injector with only 0.15 mm nozzles may not be able to provide enough fuel to the engine, the combination of the small nozzles for starting the ignition and larger nozzles for the main fuel injection may provide a promising solution.

* The effect of wall friction on mass flow rate is discussed in appendix E.
4.4.2. Effects of the Swirl on Natural Gas Jet Passing Around the Glow Plug

The mesh generator was modified to allow modeling of a glow plug in the combustion chamber. The temperature of the glow plug is set to a fixed value as the combustion wall temperature of 400 K for the simulation in this section and the next section 4.4.4 for studying the flow characteristics around the glow plug. The heat transfer model within the glow plug and from the hot glow plug to the surrounding gas will be introduced in chapter 5 and chapter 6, the glow plug ignition simulation result will be introduced in chapter 7.

Figure 4.12 shows the velocity field when methane is injected toward the glow plug with no swirl in the chamber. Vortices did not appear at the back of the glow plug, and no wake region appeared in the flow zone. This may be because its special flow characteristics compared to the conventional uniform flow over the bluff body. The injected jet is from a very small nozzle (0.5 mm diameter) impinging onto a relatively large cylinder of the glow plug (5 mm diameter), and the surrounding air is quiescent, which corresponds to a high pressure compared to the flow
at near glow plug position, which helps weakening the flow separation and vortex generation in the wake region.

![Velocity field with methane injected to the glow plug without swirl](image)

**Figure 4.12** Velocity field with methane injected to the glow plug without swirl

Different swirl intensities were tried to research the swirl effect on the jet behavior at 0° injection angle (methane injected to the central line of the glow plug). The results are shown in figure 4.13. The higher the swirl increases, the better the fuel air mixing is downstream, which corresponds to a larger area of the flammable region ($\phi = 0.5\sim1.5$). At the regular swirl ratio of 4000 rpm, the glow plug was still immersed into the core of the methane jet, which will prevent the ignition of the methane fuel. To locate the glow plug at the flammable region of the jet, an injection angle not on the central line of the glow plug is necessary.
Several jet injection angles were tested with different swirl ratios. At the back of the glow plug, there is an attachment phenomenon after the flow passes the glow plug, which helps to increase the flammable region around the glow plug and increase the mixture’s residence time in the glow plug vicinity. Both enhance auto ignition.

Previous experimental results at ERDL showed that under a regular swirl, an injection angle of 15° to the glow plug center axis in the direction upstream to the swirl is the best position for auto ignition in terms of shorter ignition delay and better combustion stability. From the simulation, the glow plug placed downstream to the swirl gives a larger flammable region around the glow plug. This is also confirmed by Tang’s simulations [1997]. But as the swirl changes, there may be more of the cold jet impinging on the glow plug and cooling it. It may even submerge the glow plug in the rich-fuel region of the jet core area. In that case, the stability of the combustion may not be good and, because of the cooling effects of the jet on the glow plug, the ignition delay may be worse (Figure 4.14). As the temperature of the glow plug is set to a fixed value of 400 K in this simulation, the cold jet effects on its temperature change cannot be shown. After the new glow plug model is developed, additional ignition simulations of an
injection angle of 15° to the glow plug center axis in the direction upstream to the swirl are conducted to compare to the experimental data in chapter 7.

![Figure 4.14 The profiles of fuel air equivalence ratio (φ) for two different glow plug locations. Left: 15° upstream, 4.182 ms after injection; right: 25° downstream, 2.135 ms after injection.](image)

4.4.3. Flow Features Over the Shielded Glow Plug

Addition of a shield around or before the glow plug is proven to reduce ignition delay by locally holding the fuel air mixture to increase the residential time, and thus increase the heat transfer [Aesoy and Valland, 1996; Fukuda _et al._, 1993; Ikeda _et al._, 1995]. It can also prevent the glow plug from being directly exposed to the cold surrounding swirling air, which will help maintain the glow plug at a higher temperature. In addition, the use of a shield can reduce the inconsistency of the natural gas ignition arising from different air swirl velocities at different engine working conditions, therefore increasing the combustion stability.

An endeavor was made to generate the mesh structure of a glow plug with a shield surrounding it (figure 4.15) the same as the experimental setup. The shield has a round slit over
the surface. The jet was injected from the nozzle at $\alpha = 28.6^\circ$ downstream from the glow plug, and the slit was turned at an angle of $\beta = 40.7^\circ$ towards the jet as shown in figure 4.16, so that only part of the jet will be induced into the shield and fed to the glow plug, while the main body of the jet keeps on penetrating outside of the shield into the combustion chamber.

Many modifications were made in both the mesh generator and the KIVA main code as listed in appendix A. This shows the capability of the KIVA code to deal with relatively complicated geometry after the necessary modifications. Thus, it should be possible to avoid having to combine other mesh generation techniques with the KIVA main code.

Figure 4.15  The illustration of the mesh structure for the shield surrounding the glow plug. The jet injected at $28.6^\circ$ downstream from the glow plug and the opening turned $40.7^\circ$ towards the jet.

Figure 4.16 shows the velocity profile near the shielded glow plug region. The base of velocity vector length scale has to be chosen very large in order to see the low velocity vectors. This figure shows that the flow inside the shield has a much slower velocity (about 20 m/s) around the glow plug compared to directly feeding the jet to a bare glow plug (about 70 m/s). Thus the gas trapped by the shield has a longer residence time near the hot glow plug. At the
same time, the flammable region attached to the glow plug is much larger than the one attached to a bare glow plug.

![Velocity profile near at the vicinity of the glow plug inside the shield.](image)

Figure 4.16  Velocity profile near at the vicinity of the glow plug inside the shield.

The fuel-air equivalence ratio within the shield is shown as in figure 4.17 for the time after injection of 0.5 ms, 1.0 ms, 1.7 ms, and 3.1ms. At time of 0.5 ms, fuel has entered inside the shield and just reached the glow plug. As from the time of 0.5 ms to the time of 3.1 ms, the front flammable region of the jet attaching to the glow plug almost did not move, while the back attachment position of the flammable region to the glow plug moved backwards. This provided a
very good sign that at the front attachment position, the flammable mixture had a long residence
time contacting the hot glow plug and thus may be able to achieve ignition. The ignition
simulation results that will be presented in chapter 7 support this conclusion.

Figure 4.17 Fuel air equivalence ratio surrounding the glow plug within a shield at different
times after the injector starts
4.5 **Comparison of Poppet Valve Model to the Models of Pressure Boundary Condition and Velocity Boundary Condition**

A comparison of new poppet valve model to the conventional velocity boundary condition and pressure boundary condition was conducted for the flow characteristics around the glow plug. The nozzle diameter was chosen as 0.5 mm, and the jet was directly impinging onto the glow plug as illustrated in figure 4.18. Three points were chosen to evaluate flow parameters adjacent to glow plug: front position of point A, upstream side position of point B, and back position of point C.

![Figure 4.18 Illustration of the simulation orientation and three locations chosen on the surface of the glow plug.](image)

4.5.1 **Cumulative Fuel and the Transient Mass Flow Rate**

Figure 4.19 shows the cumulative fuel curves flowing into the system for velocity boundary condition and pressure boundary condition, which are also the cumulative fuel curves injected into the combustion chamber.
Figure 4.19  Cumulative fuel curves for velocity boundary condition and pressure boundary condition.

From the figure, cumulative fuel flowing into the system linearly increases for both of the velocity and pressure boundary conditions. They reach the steady state at the beginning of the injection without any delay. Two curves lie in the same line with the same slope, which physically represents the same mass flow rates.

As comparison to figure 4.19, figure 4.20 shows the three cumulative fuel curves for the poppet valve model: a) total cumulative fuel flowing into the system through the valve; b) cumulative fuel in the injector; c) cumulative fuel flow into the combustion chamber. The first one is the summation of the last two values. Time starts from the opening of the valve.
To better understand the poppet valve model, an equivalent schematic piping flow chart is shown in figure 4.21.

![Diagram of poppet valve model](image)

**Figure 4.21**  Equivalent piping schematic for the flow chart of poppet valve model

This schematic has two constraints for the flow, one is the lift of the poppet valve, which is represented as a variable control valve with changeable flow area; the other is the nozzle, which is represented as a fixed restriction area valve. At the beginning of the flow, the variable valve opens gradually, fuel flows into the injector sac volume and builds up the pressure inside. During this time, the overall flow is controlled by the variable control valve – the poppet valve. When the pressure in the injector sac volume has built to a certain value, the flow exits through
the fixed valve into the combustion chamber. During this period, the flow was constrained by the fixed valve – the nozzle. The poppet valve models the physics of this flow process.

From figure 4.20, within the valve opening time from 0 to 0.1 ms, as the valve lift increases, fuel first flows into the injector with a high mass flow rate, but most of the fuel stays inside the injector sac volume and builds up the pressure inside. Fuel then flows into the combustion bomb with a delay time, the mass flow rate into the combustion chamber is first small then gradually increases until the flow reaches steady state. At the steady state, the fuel inside the injector becomes constant, and all the fuel flowing through the valve is injected into the combustion chamber through the nozzle, i.e., the total mass flow rate into the system becomes the same as the mass flow rate into the combustion chamber.

To clearly show the timing of transient process at the early stage of the injection for the poppet valve model, the derivatives of the cumulative fuel curves were calculated and plotted in figure 4.22, which physically represents the transient mass flow rates.

![Figure 4.22 Derivatives of cumulative fuel curves (transient mass flow rate) for poppet valve model.](image)
Figure 4.22 shows that at the beginning of the injector valve opening, the mass flow rate of the total fuel is very high compared to the steady state one. The mass flow rate of the cumulative fuel in the injector is the same as that of the total fuel, which implies all fuel is filling the injector until 0.35 ms. Before 0.35 ms, the mass flow rate of the fuel into combustion chamber is effectively zero. After this time, fuel starts to inject into the combustion chamber with a small mass flow rate. However, this mass flow rate first increases quickly to 71% of the steady value at about 0.1 ms, and then it keeps on increasing slowing until reaching steady state at about 0.75 ms.

The derivative figure also shows that there is a strong oscillation during the early injection stage before the flow reaches steady at 0.75 ms. The amplitude of the oscillation is first strong then damped away. This is because the pressure is also oscillating as shown in figure 4.23. For the first oscillation, even a slight backflow occurs for a short period at about the time of 0.1 ms due to this strong oscillation. The same time period for the oscillation suggests the oscillation is more reasonable to be a physical process of resonation than a computational instability. The oscillation period is 0.071 ms, which corresponds to 10485 Hz.
Figure 4.23  Pressure oscillation at point A which is just above the poppet valve top surface.

In order to compare the poppet valve model with the velocity and pressure boundary conditions, the cumulative fuel curve for the total fuel into the system was imposed onto cumulative fuel curves for the velocity and pressure boundary condition, so that their steady states lie in the same line as illustrated in figure 4.24.

Figure 4.24  Comparison of total cumulative fuel into system for poppet valve model to the ones for velocity and pressure boundary conditions.
From this figure it can be found that the three curves lie in the same line at near the steady states, implying that these three models have the same mass flow rate when they reach the steady state, although initially there is oscillation for the poppet valve model. However, before the mass flow rate for the total fuel into the system has the trend of reaching steady state for the poppet valve model, the valve has already been opened for 0.074 ms. Within this 0.074 ms, fuel flows into the system of the poppet valve model with a higher mass flow rate. Most of the fuel flowing into the system stays inside the injector to build up its pressure. As it is introduced in figure 4.22, there is already a little portion of the fuel starting to flow inside the combustion chamber at 0.035 ms after injection. This portion of the fuel into the combustion chamber before 0.074 ms is only 5.3% of the total fuel flowing into the system, the other remains in the injector, which is the 65% of the fuel in the injector when it reaches steady after 0.75 ms. So this period of time (0.074ms) is called the injector quick filling period. After this time until 0.75 ms of injection reaching steady state, it is called the injector slow filling period. Within injector slow filling period, the mass flow rate of the total fuel into the system approaches to the steady state value, which is the same as those of velocity and pressure boundary conditions. Within this period, the fuel in the injector slowly increases until it reaches a steady state of a constant value, and the other fuel injects into the combustion chamber with an increasing mass flow rate until it reaches a constant value, which is also the same as total fuel flow rate.

Both of the injector fast filling period and injector slow filling period make up the transient stage at early injection (within 0.75 ms), where the typical total injection duration is 2~4 ms.
Figure 4.25 shows the comparison of cumulative fuel into combustion chamber for poppet valve model to the ones for velocity and pressure boundary conditions. The poppet valve curve was offset for 0.35 ms so that at time zero the fuel starts injecting into the combustion chamber for all of the three models. This figure clearly shows that there is less fuel flowing into the combustion chamber for the poppet valve model compared to velocity and pressure boundary conditions because at the beginning of injection, the mass flow rate is small for the poppet valve model since the flow was not fully developed yet within the injector. The final cumulative fuel difference between these models is 0.66 mg.

In summary, the poppet valve model considers the transient process for fuel injection of the early stage (0.75ms), which consists of injector fast opening and injection slow injection periods. As a contrast, the velocity and pressure boundary conditions neglect this transient injection process. For the poppet valve model, a low mass flow rate for the fuel injecting into the combustion chamber at the beginning of the injection makes the jet momentum low, thus resulting in poor mixing with air and taking longer time to reach the glow plug compared to the
velocity and pressure boundary conditions. This may make the ignition delay time longer for the poppet valve model. So, velocity and pressure boundary conditions may under-estimate the ignition delay time.

4.5.2. Parameters of the Jets When Reaching Glow Plug

Figure 4.26 shows the comparison of the parameters when jet reaches the glow plug surface at point A for velocity boundary condition, pressure boundary condition, and poppet valve model. From this figure it can be seen that velocity boundary condition and pressure boundary condition have the similar flow parameters when the jets reach the glow plug, but they are quite different with the poppet valve model. Besides the temperatures are almost same for the three models, the velocities and time for the jet to reach the glow plug surface point A are much different. Velocities are 22 m/s for velocity BC and 19 m/s for pressure BC compared to 31 m/s for poppet valve model. The time of jet reaching glow plug is: 0.026 ms for velocity BC and 0.023 ms for pressure BC compared to 0.048 ms for poppet valve model.

For the poppet valve model compared to the velocity and pressure boundary conditions, the higher gas velocity when reaching the glow plug implies more cooling effect by the cold jet to the hot glow plug. The longer time for the gas jet to reach the glow plug implies a longer physical delay time for ignition before the jet reaches glow plug. Both of these two reasons may result that the ignition delay time for poppet valve model should be longer than those of the velocity BC and pressure BC, i.e. the velocity BC and pressure BC may under-estimate the ignition delay time compared to the poppet valve model.
4.5.3. **History of Fuel Air Equivalence Ratio at Different Locations on Glow Plug Surface**

Figure 4.27 shows the history of fuel air equivalence ratio development in the gas cells adjacent to three different locations at the glow plug surface: point A, point B, and point C for the three models. Fuel air equivalence ratio is a parameter directly affecting the ignition delay time. From this figure it can be seen that the velocity BC and the pressure BC have similar results compared to each other, but their results are very different from that of the poppet valve model. There is a delay time for the development of fuel air equivalence ratio between the poppet valve model compared to the velocity BC and the pressure BC. This is because it takes time for the poppet valve model to first pressurize the sac volume and develop the internal flow within the injector. Also, the initial gas flow from the injector has lower momentum. These differences imply the under-estimation of ignition delay time for the velocity and pressure boundary conditions.
(a) Fuel air equivalence ratio history at point A for three models

(b) Fuel air equivalence ratio history at point B for three models

(c) Fuel air equivalence ratio history at point C for three models

Figure 4.27 Fuel air equivalence ratio history at three different points on the glow plug for three models.
The poppet valve model has a significant difference compared to the conventional velocity and pressure boundary conditions, which neglect the process of the internal flow development within the injector, thus may under-estimate the ignition delay time. This conclusion is confirmed in chapter 7 by using the glow plug ignition model to simulate ignition process for the velocity BC, the pressure BC and the poppet valve model.

4.5.4. Comparison of Ignition Delay Time

Simulations of ignition delay for the comparison of poppet valve model to velocity boundary condition and pressure boundary condition were conducted using glow plug ignition model, this model will be introduced later in chapter 5 and 6.

The ignition simulation was conducted for a jet injected from a small nozzle impinging onto a bare glow plug with an angle to the jet. The detailed configuration and the simulation results for ignition and combustion for poppet valve model are shown in section 7.1.

Table 4.5 tabulates the simulation results of ignition delay for the three models. The velocity pressure boundary condition and pressure boundary condition have almost the same simulation results because of their similar flow characteristics as discussed above. However, the ignition delay time for poppet valve model is 20% longer than the velocity and pressure boundary conditions as expected with the reasons analyzed earlier in this section. The ignition delay from the poppet valve simulation is much closer to the experimental results [Fabbroni, 2004].
Table 4.5  Simulation results of ignition delay for three models

<table>
<thead>
<tr>
<th>Cases</th>
<th>Velocity BC</th>
<th>Pressure BC</th>
<th>Poppet Valve Model</th>
<th>Experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ignition delay</td>
<td>1.41 ms</td>
<td>1.40 ms</td>
<td>1.76 ms</td>
<td>1.75 ms</td>
</tr>
</tbody>
</table>

As a conclusion, velocity and pressure boundary conditions generate a steady state jet flow from the beginning of the injection. The poppet valve model has the similar steady state flow characteristics with velocity and pressure boundary conditions after the injection reaches steady after 0.8 ms. However, during the transient state for the early stage of the injection, the poppet valve model has significant differences with velocity and pressure boundary condition in flow parameters, such as time for the jet to reach the glow plug, velocity when jet reaching the glow plug, the historical change of fuel-air equivalence ratio near glow plug surface, the transient mass flow rate. These flow parameters are the important factors affecting the ignition delay time, thus the transient state differences result the different ignition delay for the poppet valve model compared to the velocity and pressure boundary conditions.

Some of the researchers improved velocity boundary conditions using a spatially-predetermined velocity profile with a temporally-varying velocity history from an experimental results library [Ouellette et al., 1998; Ouellette and Hill, 2002; Li et al., 2005]. The improved velocity boundary condition considers this transient change of the real injection process. However, with a new injector design or if experimental data is lacking, the poppet valve model provides the possibility of studying the flow characteristics in the injector and combustion chamber and the design parameters of the new injector.
4.6 Summary

This chapter addressed one of the difficulties of the DING engine - the behavior of the natural gas injector, and presented simulation results that accurately accounts for the transient flow characteristics of a real injector. The results obtained provide much improved boundary conditions for modeling the subsequent ignition process.

The following chapter addresses the second difficulty of the DING engine - ignition - by presenting a new model of glow plug thermal behavior.
Chapter 5

Glow Plug Discretized Model

As noted in chapter 2, one technical difficulty for DING engine research is that there is currently no proper glow plug model. This chapter introduces the first discretized glow plug model developed to research the physics of glow plug transient performance for ignition assistance in a direct injected natural gas (DING) engine.

The simplest thermal model, treating the glow plug as a lumped heat capacitance with a uniform temperature, is not suitable for glow plug transient research since both experimental data and theoretical analysis show the thickness of the heat penetration layer is very small (~10^{-5} m) within the time scale of the ignition preparation period (1~2 ms).

Discretization has to be applied to the solid glow plug domain. A simplified heat transfer model was set up within the discretized glow plug in order to save computational time especially for coupling with the surrounding gas domain in the KIVA-3V code. The axial conduction heat loss to the base and radiation loss were also taken into consideration.
The new glow plug discretized model reveals the physics of the glow plug transient heat transfer with the surrounding gas that occurs within a small heat penetration thickness. This model used together with the virtual gas sub-layer model to be introduced in chapter 6 successfully simulates the natural gas ignition process for the DING engine, and can provide detailed information about the glow plug local temperature distribution which is essential for glow plug life time design.

5.1. Introduction to Glow Plugs

One of the most difficult technical challenges for direct injection natural gas (DING) engine is that of natural gas ignition due to the high spontaneous ignition temperature of methane, inadequate mixing with air, and low injection temperature during the injection process. An ignition assist method, such as pilot fuel, spark plug, etc., has to be used in order to achieve short and stable ignition. In this research, a glow plug is used to assist natural gas ignition.

5.1.1. Glow Plug Structure

![Figure 5.1 Structure details of the sheathed type glow plug](www.NGK.de)

The glow plug chosen in the experiments is a sheathed type glow plug from NGK Spark Plug Co. Ltd, which consists of an outer protective tube, the heating element consisting of heating and control coils embedded in electrical insulating powder, and connection and mounting...
features, is shown in figure 5.1 [www.NGK.de]. Representative dimensions of the heater tube are 5 mm dia. × 24 mm length with a thickness of 0.7 mm. The glow plug has a 12 mm thread on the body, and its total length is about 90 mm. The heating and control coil is packed in a compacted, electrically insulating ceramic powder (magnesium oxide) with a very high heat conductivity. The powder is highly pressed together during mechanical compaction, so that the coil sits absolutely firmly to ensure high thermal conductivity and withstanding all vibrations.

Since the glow plug has significant heat capacitance, it takes time to heat up and cool down when initially energized or powered off respectively. From the manufacturer’s specifications, the delay time of pre-heating process for the standard type of the glow plug is 20~25 seconds from common room temperature to 800°C in still air as shown in figure 5.2 [www.NGK.de].

5.1.2. Glow Plug Environment in an Engine

In the engine environment, a glow plug is immersed in the gaseous contents of the engine cylinder, primarily air until ignition and products of combustion after ignition. During an engine cycle, the composition, temperature, pressure and velocity of the gases surrounding the glow plug are continually changing. Thus, while the heating element is continually powered, the heating tube surface experiences convective cooling and heating that varies as the engine cycle progresses. During the intake stroke, the glow plug is cooled by incoming air. It is also cooled by
the high velocity injected natural gas, which is much cooler than the in-cylinder compressed air at the time of injection. Finally, the glow plug is heated by hot products of combustion after ignition occurs. Note that the heating and cooling are out of phase with the requirements for ignition. Ideally, the glow plug surface temperature would be the hottest during injection to facilitate ignition but in practice its temperature falls due to cooling by the cold natural gas jet. The heating by hot combustion products mainly results in high temperatures that limit the lifetime of the glow plug.

A model of glow plug surface temperature variation during an engine cycle is necessary to effectively simulate hot surface ignition in the direct injection natural gas engine. A first step was to calculate the Biot number for the convective cooling where the glow plug is considered to be a cylinder in crossflow. The Hilpert correlation for Nusselt number was used [Incropera and deWitt, 1996]. The Biot number is a dimensionless number relating the heat transfer resistance inside and at the surface of a body. It is defined as:

\[
Bi = \frac{hL_c}{k}
\]

where: \( h \) is the convective heat transfer coefficient;

\( L_c \) is the characteristic length;

\( k \) is the thermal conductivity of the solid body.

Two situations were evaluated: cooling by intake air and cooling by injected methane jet as summarized in table 5.1. The detailed calculation can be found in Appendix F.1.
Table 5.1  The conditions used to calculate the Biot number

<table>
<thead>
<tr>
<th>Case</th>
<th>Velocity</th>
<th>Temperature</th>
<th>Pressure</th>
<th>Re_D</th>
<th>Biot</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake air cooling</td>
<td>8 m/s</td>
<td>300 K</td>
<td>101 kPa</td>
<td>524</td>
<td>0.0034</td>
</tr>
<tr>
<td>Injected gas cooling</td>
<td>52 m/s</td>
<td>683 K</td>
<td>4 MPa</td>
<td>129,327</td>
<td>0.109</td>
</tr>
<tr>
<td>With 0.34 mm dia. nozzle</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Injected gas cooling</td>
<td>92 m/s</td>
<td>627 K</td>
<td>4 MPa</td>
<td>258,666</td>
<td>0.185</td>
</tr>
<tr>
<td>With 0.50 mm dia. nozzle</td>
<td></td>
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</tr>
</tbody>
</table>

5.1.3. Defaults of Lumped Heat Capacitance Methods for Glow Plug Modeling

Although this simple calculation returns a Biot number value in the range that may be treated as a lumped capacitance (Bi ≤ 0.1), the glow plug cannot be treated as a lumped capacitance because the heat transfer situation is far more complex, with internal heat generation and both surface radiation and axial conduction occurring in addition to convection. As well, the ignition preparation process occurs over a very small time scale (10⁻³~10⁻¹ s). The Fourier number ($Fo$) is a dimensionless time scale for transient heat transfer. It is defined as [Incropera and deWitt, 1996]:

$$Fo = \frac{\alpha \cdot t}{L_c}$$

where: $\alpha$ is thermal diffusivity;

$L_c$ is the characteristic length;

$t$ is the elapsing time during the process.
In either of the cases listed above, $Fo \sim 10^{-4}$ to $10^{-3}$, which indicates that the surface response to the rapid changes in the surrounding gaseous environment correspond to a very early regime of transient heat transfer.

The early regime with small heat penetration thickness implies that the simple lumped heat capacitance of the glow plug is not suitable to model the process of glow plug heating of the surrounding gas and igniting the mixture.

An improved lumped heat capacitance model of the glow plug was then proposed to compensate for the small heat penetration thickness. It is designed to use the variable heat capacity of the material within the changing penetration thickness $\delta$ as time elapses. This improved lumped heat capacitance model still could not work well after many efforts. Since the penetration thickness $\delta$ is changing from the glow plug surface, it makes the model hard to implement. The internal heat source at the glow plug center is especially hard to apply because of the moving boundary of the penetration thickness. In addition to these difficulties, more importantly the improved lumped heat capacitance model gives a uniform temperature on the surface of the glow plug, which implies that as the cold natural gas jet impinges onto the part of the glow plug surface, the drop of the spatially uniform surface temperature will make the ignition extremely difficult to occur. In reality, after the cold natural gas jet reaches the glow plug, the temperature of the impinged surface of the glow plug will drop, but the other areas of the glow plug surface and their surrounding gas still remain at high temperature. This remaining high temperature surface area will ignite the flammable mixture at the some particular positions on the glow plug.
From the above analysis, it can be concluded that the glow plug has to be discretized so as to consider both spatial and temporal dependence in the ignition process.

5.2. Experiments on Glow Plug Transient Response Time

5.2.1. Experimental Setup

Some experiments were designed and conducted to evaluate the delay time between the surface and the core temperature of the glow plug, as well as the transient processes of glow plug start-up, turn-off, and other dynamic changes.

The glow plug was fixed in still air and powered by a nominal 5V electrical source to reach temperature equilibrium at a pre-determined power. Three s-type thin thermocouples were placed in contact with the surface of the glow plug to measure the surface temperature. Their distances from the tip of the glow plug are: 2.5 mm for \( T_1 \), 12 mm for \( T_2 \), and 20.5 mm for \( T_3 \). The voltage \( V \) and current \( I \) applied on the glow plug were recorded to monitor the glow plug core temperature by calculating the glow plug electrical resistance, since the electrical resistance was reported to have a linear relationship with the glow plug core temperature [Abate, 2001]. An air gun was used to blow room temperature compressed air onto the glow plug to make it cool down quickly by providing forced convection. The systematic diagram of the experiment is shown in figure 5.3.
5.2.2. Response Delay Time Between Surface Temperature and Core Temperature

After the glow plug reached a steady state in still air, an air gun was used to blow compressed air onto the glow plug and cool it down quickly. Figure 5.4 shows the delay of the response time between the core temperature dropping and surface temperature dropping of the glow plug. The average delay time is $0.415 \pm 0.046$ s with 95% confidence from 4 experiments. This can be interpreted as: after the surface temperature of the glow plug is cooling down, it takes about 0.42 s for the core of the glow plug with radius of 2.5 mm to sense the cooling effect. For comparison of time scales, an engine cycle at 1800 rpm takes 0.067 s, so we can deduce that during the early regime ($\sim 10^{-4}$ s) of the glow plug temperature changing process, the penetration thickness should be very small, and that during the course of an engine cycle the core temperature should not change much.

![Temperature Delay from Surface to Core for Glow Plug](image)

Figure 5.4  Delay time of the core temperature compared to the surface temperature of the glow plug. The glow plug power was 43W in still air initially.
5.2.3. Difference of The Transient Processes Between Start-up and Dynamic Change

Figure 5.5 shows the start-up and turn-off processes of a glow plug which is powered at 43 W. After the glow plug is turned on, the resistance of the glow plug heating element reaches a steady value at about 16 s. The resistance represents the core temperature of the glow plug. They have a linear relationship from Abate’s correlation [Abate, 2001]. Finally the surface temperature $T_1$ reaches a steady value of 950 K at about 25 s from the initial 298 K, corresponding to a 9 s delay compared to the core temperature. This result shows good agreement with the manufacturer’s data as shown in figure 5.2. This process duration is relatively long and it occurs in static surroundings, thus it can be treated as a late regime where the lumped heat capacitance model may be applied.

Figure 5.6 shows the dynamic change of the glow plug temperature by using the air gun blowing compressed air onto the glow plug for 1.6 seconds. This time period is much longer than the time of the engine intake process (0.125 s for a 4 stroke engine running at 240 rpm), which is similar to the cooling effect on the glow plug by the intake fresh air in engine application. After

![Figure 5.5 The transient process of the glow plug power-on and turn-off.](image1)

![Figure 5.6 The transient process of the glow plug temperature dynamic change.](image2)
the air gun stops blowing air, the surface temperature of the glow plug will recover within 1.4 s. While the time scale of this process is two orders of magnitude longer, it is similar in concept to the convective cooling of the ignition preparation period. These processes are relatively short especially in the engine application (in ms), and experience a dynamically changing surroundings. Thus they can only be analyzed as early regime.

The experimental results are listed and compared in the table 5.2.

Table 5.2 Comparison of static power-on process and dynamic cooling/heating process.

<table>
<thead>
<tr>
<th>Event</th>
<th>Position</th>
<th>Stage 1</th>
<th>Stage 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Temp. change</td>
<td>Time duration</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(K)</td>
<td>(s)</td>
</tr>
<tr>
<td>Dynamic cooling</td>
<td>Core</td>
<td>1430→1390</td>
<td>1.4</td>
</tr>
<tr>
<td></td>
<td>Surface</td>
<td>948→763</td>
<td>0.7</td>
</tr>
<tr>
<td>Dynamic heating</td>
<td>Core</td>
<td>1390→1430</td>
<td>6.1</td>
</tr>
<tr>
<td></td>
<td>Surface</td>
<td>711→923</td>
<td>1.4</td>
</tr>
<tr>
<td>Static power-on</td>
<td>Core</td>
<td>296→1203</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>Surface T₁</td>
<td>296→859</td>
<td>12</td>
</tr>
</tbody>
</table>

For the dynamic cooling process, the glow plug surface temperature drops a total of 237 K, first decreasing at a very fast rate of 263.4 K/s and then slowing down at a rate of 74.6 K/s. In contrast, the core temperature (resistance) only drops 40 K with a fairly steady slow rate at 28.6 K/s. Our glow plug discretized model reveals that this small change of the core temperature is because of the delay of the penetration, the inertia of the heat capacity, and the continuous source power at the core position of the glow plug.

Similarly for the dynamic heating process, the glow plug surface temperature recovers a total of 239 K, first increasing at a very fast speed of 151 K/s and then slowing down at a speed of 4.1 K/s, because the temperature gradient is smaller between the core and surface of the glow plug.
plug. In contrast, the core temperature (resistance) recovers 40 K with a fairly steady slow rate at 6.6 K/s. The dynamic processes imply that the large temperature decrease only happens at the outside very thin layer of the glow plug, but not into the core region of the glow plug.

Comparing the dynamic heating process to the glow plug startup process, it takes 1.4 s and 10.0 s correspondingly for the surface temperature to increase from 711 K to 923 K. This is because for dynamic process, the temperature at only the outside thin layer of the glow plug decreases, but most of the inside part of the glow plug remains at the high temperature. Furthermore, the inner part acts as a heat source making the outer cool layer recover the higher temperature quicker. However, for the startup process, even though the core temperature quickly becomes higher than the surface temperature since the heat source is at the core position, all of the glow plug is initially at a low temperature. So the glow plug needs a much longer time to heat up to the same temperature.

As a conclusion from the experiment, the dynamic temperature change of the glow plug in the engine application within a short time will only make the very thin outer layer of the glow plug change temperature, and the penetration thickness is relatively very small. This requires that any study on the glow plug temperature dynamic change has to discretize the glow plug to very thin outer layers.

### 5.3. Radiation Heat Loss and Conduction Heat Loss

When the power is turned off, it takes about 30 seconds for the surface temperature to decrease from 970 K to 410 K in still air. From the theoretical analysis of a lumped heat capacitance model with only natural convection, the governing equation is [Incropera and deWitt, 1996]:

\[
\]
\[ T - T_\infty = (T_i - T_\infty) \cdot \exp(-Bi \cdot Fo) \]  \hspace{1cm} \text{Equation (5-1)}

where: \( T_\infty \) is the surrounding air temperature;

\( T_i \) is the initial temperature of the glow plug;

\( Bi \) is the Biot number;

\( Fo \) is the Fourier number.

The analytical result shows that the temperature can only drop to 656 K within 30 s; this indicates the glow plug surface radiation must play a non-negligible role. The detailed analytical calculation can be found in Appendix F.2.

The heat loss from the radiation can be evaluated from the equation:

\[ q = \varepsilon A \sigma (T_s^4 - T_{\text{sur}}^4) \]  \hspace{1cm} \text{Equation (5-2)}

where: \( T_s \) is the surface temperature of the glow plug;

\( T_{\text{sur}} \) is the surrounding temperature of the combustion bomb wall;

\( \varepsilon \) is the emissivity of the glow plug.

\( A \) is the surface area of the glow plug;

\( \sigma \) is the Stefan-Boltzmann constant, \( 5.670 \times 10^{-8} \) W·m\(^{-2}\)·K\(^{-4}\)

Taking the surface temperature \( T_s = 950 \) K and the surrounding temperature \( T_{\text{sur}} = 300 \) K, the heat loss rate from radiation is about 10.2 W at steady state. In the engine application, the radiation loss will be higher since the surface temperature of glow plug is higher when powered at 100 W under the engine operation, although this would be offset somewhat by \( T_{\text{sur}} \) being higher.
The heat conduction loss through the glow plug body to the supporting base can be evaluated as about 6.2W from $T_2$ and $T_3$ and their distance in figure 5.5 at a steady 43 W power input, and about 3.8 W at 25 W power input. In the engine application, we can estimate the conduction heat loss from the glow plug to the combustion chamber is in the range of 10-12W since the power is at 100 W and the base of the glow plug is at 400 K.

5.4. Theoretical Analysis of Heat Penetration Thickness in Early Regime

When a long cylindrical solid body initially at high temperature of $T_i$ is exposed to a cold temperature environment, suppose that its surface temperature drops down to $T_0$. The solid body will keep losing heat to its surrounding cold environment, and the penetration layer will grow towards the inside as shown in figure 5.7.

Assuming the solid body is infinitely long, and using a 1-d simplified heat transfer equation, the penetration thickness $\delta$ can be derived as [Incropera and deWitt, 1996]:

$$\delta \sim (\alpha \cdot t)^{1/2}$$  \hspace{1cm} \text{Equation (5-3)}$$

where: $\alpha$ is the thermal diffusivity of the glow plug, $\alpha = \frac{k}{\rho \cdot c_p} = 3.08 \times 10^{-6}$ m$^2$/s.

$k$, $\rho$, $c_p$ are the glow plug thermal conductivity, density and specific heat, respectively.

For the glow plug used in this research, the outer shell material is an alloy of Inconel 601, and the thickness of the shell is about 0.7 mm. In the combustion chamber computation, the time step is $10^{-7} \sim 10^{-6}$
s. At the early regime of the glow plug initially heating up the surrounding air, the time scale between the natural gas injection to the natural gas front reaching the glow plug is on the order of $10^{-5} \sim 10^{-4}$ s (10-100 µs) depending on different locations and layouts of the glow plug and its surrounding shield. This time corresponds to $\delta = 5.55 \sim 17.55 \times 10^{-6}$ m, which means that the heat penetration thickness $\delta <<$ shell thickness $= 1 \times 10^{-3}$ m.

Furthermore, by equation (5-3), it can be derived that it takes about 160 ms to penetrate through the 0.7 mm thickness of heater tube, which is longer than the total combustion and expansion process of 130 ms if the engine runs at 230 rpm in the experiments. This implies that within the combustion process, the heat penetration thickness will be not beyond the thickness of the outer shell heater tube.

The small heat penetration thickness implies that we cannot use the simple lumped heat capacitance of the glow plug to model the process of glow plug heating of the surrounding gas and igniting the mixture. The glow plug has to be discretized so as to solve the above discussed issues.

### 5.5. Glow Plug Discretization

A new model needs to be set up to discretize the glow plug shell in order to have the right response inside the glow plug to the temperature change. This model for the glow plug also needs to be incorporated with the surrounding KIVA-3V gaseous cells by the connection of heat transfer. Based on the analysis of penetration thickness, the proper thickness of the discretized glow plug grids need to be small enough to reflect the penetration thickness changes in the early regime. In the computation, the optimized thickness is at the scale of $10^{-6}$ m, which gives 700
layers for the entire 0.7 mm thickness of the glow plug outer shell. To incorporate the model with the surrounding KIVA-3V gaseous cells, it is more convenient to set the cell surface of the glow plug to be the same as the surrounding gaseous cell surface. This requires total of 36×30×700=756,000 cells for the glow plug.

To reasonably simplify the glow plug discretization model, the following two assumptions were implemented to save computational time and storage, based on the geometry of the glow plug and its discretized cells as shown in figure 5.8.

1. Within the solid glow plug cells, there is only heat conduction in the \( r \) direction of the cylindrical coordinates, which is vertical to the glow plug surface from the inner layer to the outer layer (or vice versa). The heat transfer is negligible in the \( \theta \) and \( z \) directions which are parallel to the glow plug surface.

This simplification is based on the fact that the effective heat transfer surface areas of the cells in \( r \)-direction are 120~1750 times larger than the ones in \( \theta \) or \( z \) directions (this range is because the improved uneven mesh structure was implemented in the KIVA-3V mesh generator), so the heat transfer from the inner layer to the outer layer direction dominates.

2. The cylindrical cell layer can be simplified to have the shape of a flat plate.

The cylindrical glow plug generates an outer surface area slightly greater than the inner surface area of each solid cell in the layer. But because the penetration thickness and the thickness of each layer of the glow plug is very small, the ratio of the layer thickness to the radius of the glow plug is: 4.0×10^{-4}, the curvature of the cell can be neglected and the inner and outer layer can be treated as the same area.
From the above two assumptions, we can develop a simplified quasi-3d glow plug discretized model, which allows a non-uniform temperature distribution on the 2-d surface of the glow plug, with a different temperature profile over the inner thickness of the glow plug. Figure 5.9 shows one heat transfer channel of the glow plug and the initial temperature profile within the channel.
To take the conduction loss into consideration while keeping the glow plug model simple, the effective internal heating power is estimated as the total electric power (100 W), less the conduction loss of 10 W (about 10%). Assuming that the glow plug is at steady state at the start of the computation, which makes the effective heating source of the glow plug equivalent to a proper slope of the temperature profile along the depth into the inner layers from the outer layer temperature of about 1300 K from the previous experimental data [Abate, 2001; Fabbroni, 2002] until it reaches the glow plug inner shell boundary of 0.7 mm. This 0.7 mm thickness will allow about 0.16 seconds of the computation before penetrating to the boundary of the inner layer, which is much more than duration of the ignition process time (less than 10 ms).

The radiation loss is applied on the entire outer surface of the glow plug, since radiation only affects heat transfer on the outer layer of the glow plug.

From the initial computation of the full discretization model of the glow plug, we found that only a few of the outer layers (within 10-30 layers) of the glow plug are within the heat penetration thickness in the early regime, the other inner layers are inactive in terms of the heat transfer. The improved discretized model was then set up to accommodate this character to further lessen the computational load. It uses a variable number of active layers involved into the heat transfer calculation, and bypasses the inert heat transfer layers. The number of active layers is determined by comparing to a small threshold of temperature change of the layer for the time step. An inactive layer is added to the heat transfer calculation only when the penetration boundary reaches it.

In summary, the glow plug discretized model reveals the physics of the glow plug transient heat transfer process within a small heat penetration thickness with the surrounding gas.
After further coupling with the surrounding gaseous domain calculated by the KIVA-3V code, the discretized glow plug model can successfully simulate the natural gas ignition process at the specific location of the glow plug. It can calculate the detailed local temperature distribution at the glow plug surface, and the temperature profile along the depth into the glow plug inner layer.

The next chapter describes how the adjacent gas cells in KIVA are modified to interact with the discretized glow plug model just described.
Chapter 6

Virtual Gas Sub-Layer Model for Thin Gas Cells Surrounding the Glow Plug

The previous chapter described how the glow plug was discretized into layers of small cells. Adjacent to these small cells are the surrounding gas cells in the gaseous domain of the combustion chamber. These surrounding gas cells will exchange heat with the glow plug surface cells in the solid phase domain. This heat exchange from the solid glow plug to the surrounding gas cells provides the energy input for ignition. This chapter will study the heat exchange between adjacent solid and gas phase cells, thus researching the physics of the ignition process and modeling a key step in the ignition process.

6.1. Necessity of the Virtual Sub-Layer Model

6.1.1. Evaluation of the Dynamic Thermal Boundary Layer Thickness

Initially the glow plug outer layer is set at a high temperature of 1300 K, based on experimental data [Fabbroni, 2002], and the surrounding gas is at a relatively low temperature of
850K a the end of the compression stroke. Heat transfer will occur from the glow plug out to the surrounding gas as a result of this temperature difference. At the interface between the solid and gaseous phases, heat transfer occurs by conduction. The conduction heat transfer rate is determined as:

\[ q = \frac{k_{\text{gas}}}{\delta_{\text{gas}}} (T_{\text{gp}} - T_{\text{gas}}) \]

where:  
- \(T_{\text{gp}}\) – is surface temperature of the glow plug cell
- \(T_{\text{gas}}\) – is the temperature of the surrounding gaseous cell
- \(k_{\text{gas}}\) – is the gas thermal conductivity
- \(\delta_{\text{gas}}\) - is the thickness of the gaseous cell.

By receiving the heat transferred from glow plug, within the time period \(\Delta t\), the surrounding gas temperature is increased by \(\Delta T_{\text{gas}}\). The governing equation is:

\[ Q = q \cdot A \cdot \Delta t = m_{\text{gas}} \cdot c_{\text{pgas}} \cdot \Delta T_{\text{gas}} \]

i.e.

\[ \frac{k_{\text{gas}}}{\delta_{\text{gas}}} (T_{\text{gp}} - T_{\text{gas}}) \cdot A \cdot \Delta t = \rho_{\text{gas}} \cdot A \cdot \delta_{\text{gas}} \cdot c_{\text{pgas}} \Delta T_{\text{gas}} \]

It can be simplified as:

\[ \frac{\Delta T_{\text{gas}}}{\Delta t} = \alpha_{\text{gas}} \cdot \frac{(T_{\text{gp}} - T_{\text{gas}})}{\delta_{\text{gas}}^2} \]

Equation (6-1)

where: \(c_{\text{pgas}}\) is the heat capacity of the surrounding gas at constant pressure

\(\rho_{\text{gas}}\) is the density of the surrounding gas

\(\alpha_{\text{gas}}\) is the thermal diffusivity of the surrounding gas, \(\alpha_{\text{gas}} = \frac{k_{\text{gas}}}{\rho_{\text{gas}} c_{\text{pgas}}}\)
This shows that the rate of temperature increase of the surrounding gas is inversely proportional to the square of the gas cell thickness. If the gas cell is too thick, then it will take a longer time to be heated to high temperature, because more mass of the gas is stored in the cell and needs to be heated.

To illustrate this point, take $\delta_{\text{gas}} = 0.5 \text{ mm}$ and $(T_{\text{gp}} - T_{\text{gas}}) = (1300 \text{ K} - 850 \text{ K}) = 450 \text{ K}$ since the thickness of the gas cells near glow plug is in the order of 0.5 mm. At an initial gas temperature of 850 K, a pressure of 4 MPa, $k_{\text{gas}} = 0.058 \text{ W/m-K}$, $\rho_{\text{gas}} = 15.7 \text{ kg/m}^3$, $c_{p_{\text{gas}}} = 1.1 \text{ kJ/kg-K}$, and $\alpha_{\text{gas}} = 3.36 \times 10^{-6} \text{ m}^2/\text{s}$, then $\Delta T_{\text{gas}}/\Delta t = 6.0 \times 10^3 \text{ K/s}$.

This estimated result can be interpreted as follows: In order to increase the temperature of the 0.5 mm thickness of the surrounding gas to 1250 K, about 0.07 second will be required. As the experimental apparatus runs at 230 rpm, the total duration of the power stroke is only about 0.13 s. In order to achieve ignition, a time scale on the order of milliseconds is required. In addition, the speed of the temperature increase is based on the initial temperature difference between the glow plug and the gas surrounding it. As time elapses during the heat transfer process, this temperature difference keeps on decreasing, which makes the overall heating time much longer than the above estimated value. So the heating time will be too slow for the engine ignition application if a 0.5 mm gas layer thickness is used for estimation.

To correctly evaluate the process of heating up the gas surrounding the glow plug, the gas layers have to be much thinner than 0.5 mm. In reality, the gas layers within a few micrometers to the glow plug will be heated up near to the glow plug temperature, and the temperature drops quickly as the distance away from the glow plug wall increases, as shown in figure 6.1.
If we assume that the gas velocity will be negligible when very close to the wall (within a few micrometers distance), heat transfer between the solid wall and the surrounding gas very close to the wall can be simplified to heat conduction. Heat convection within the gas phase except for the gas very close to the wall can be carried out by the normal means of CFD by including convection terms in the mass and energy equations. The mathematical model of this heat conduction can be summarized as:

Conduction equation: \[ \frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \cdot \frac{\partial T}{\partial t} \]  
Equation (6-2)

Initial condition: \[ T = T_i \] at \[ t = 0 \]

Boundary conditions: \[ T = T_{gp} \] at \[ x = 0 \]
\[ T = T_i \] at \[ x = \infty \]

As the thermal capacity (proportional to \( \rho c_p \)) of the glow plug is much higher than the surrounding gas (210 times), the temperature change of the glow plug is a lot slower than that of the gas. So in the very early regime, we can simplify the boundary condition at \( x = 0, T_{gp} \) is a constant, where \( T_{gp} \) is the actual time averaged surface temperature of the glow plug within the early regime. The analytical solution to equation (6-2) can be derived as following [Bejan, 1993]:

\[ \frac{T_{gp} - T}{T_{gp} - T_i} = erf \left[ \frac{x}{2(\alpha_{gas} t)^{1/2}} \right] \]  
Equation (6-3)
where: \( erf(x) \) is the error function, defined as: 

\[
erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} \, dt,
\]

here \( t \) is an integral variable. The error function has the noteworthy properties: \( \text{erf}(0) = 0; \text{erf}(1) = 0.85, \text{erf}(\infty) = 1. \)

Note that this equation is only valid in the early regime of the glow plug heating up its surrounding gas for the ignition preparation period, before the jet reaches the glow plug and chemical reaction dominates. In terms of the engine application, this is also the period from the start of injection until the injected jet reaches the glow plug, which is usually within 100 µs. Within this period, the glow plug is heating the surrounding gas (about 850 K) to near its surface temperature (about 1300 K) to generate a hot gas layer in order to prepare the ignition when the methane jet mixed with air at the jet boundary reaches it. As the chemical reaction rate exponentially increases with the temperature, the layers of \( T > 1200 \text{ K} \) contribute more to the preparation of ignition.

To evaluate the thickness of the \( T > 1200 \text{ K} \) layer within a 100 µs heating-up period, take 

\[
\frac{T_{\text{sp}} - T}{T_{\text{sp}} - T_i} = \frac{1300K - 1200K}{1300K - 850K} = 0.22, \quad t = 100 \text{ µs, and } \alpha_{\text{gas}} = 3.36 \times 10^{-6} \text{ m}^2/\text{s.}
\]

The solution of the hot layer thickness is \( x = 7.3 \mu\text{m} \). This shows that only a very thin layer of the gas may be heated up to a high temperature for ignition preparation within 100 µs.

From this analysis we can see that, to achieve the correct temperature profile for the thermal boundary layers within the gas layers near to the glow plug, we have to set the gas layer to be very thin, in micrometers. This is very important in order to research the ignition of the natural gas.
6.1.2. Limitation of Conventional CFD on Small Mesh Sizes in the Thin Thermal Boundary Layers

A thin thermal boundary layer requires that the cells around the glow plug be of small size, a scale of micrometers. However, because of the limitations of mesh structure and KIVA mesh generation, the minimum thickness of the gas layer that can be generated is 0.07 mm for our particular case. Otherwise non-convex mesh will be formed because of the curvature of the glow plug, and non-convex mesh is prohibited for the KIVA code (figure 6.2).

Although for fully implicit CFD codes even a large time step can still meet stability requirement, a large marching time step will give a bigger truncation error compared to a small one for the overall transient process unless the final state is steady flow situation [Anderson, 1995]. In conventional CFD simulations, a too thin layer will also necessitate a very small time step, since the overall time step is restricted by the smallest mesh size in the whole domain. KIVA as a not fully implicit CFD code will require an extreme small time step for the thin gas layer of micrometer thickness. This would result in unaffordable computational time. However, from the above analysis, a 0.07 mm gas layer is still too big to study the time-varying surface temperature of the glow plug and ignition of the natural gas. Thus, the required scale of micrometers is unrealistic by using the conventional CFD method in terms of high computational load.

Figure 6.2 Structure of the minimum 0.07 mm thin gas layer surrounding the glow plug.
To overcome these problems, a new model of virtual multiple thin sub-layers in the gas cells surrounding the glow plug was developed.

### 6.2. Assumptions and Simplifications

To realize the thin layers of the surrounding gas of the glow plug for ignition study, the virtual sub-layer model within the surrounding gas cells was developed as shown in figure 6.3.

The initial thickness of each virtual sub-layer is selected to be the same as the thickness of the connecting glow plug cell for our study, which is a constant value arbitrarily set by program input as 3.3 µm; it can be set at other values in the range of about 1~5 µm. A total of only 4 virtual gas sub-layers were set up to reasonably represent the temperature profile near the glow plug surface while minimizing computation.

Within the very thin virtual sub-layers, the following simplifying assumptions are made:

1. Heat and mass transfer occur only by molecular diffusion but not by convection. There is redistribution of total mass between sub-layers due to the temperature increase by heat transfer. This is also redistribution of the mass of individual species due to chemical reaction.

2. Gas velocity is negligible, no convective mass flow crosses the sub-layer boundaries, so only conduction heat transfer occurs between the virtual sub-layers. The sub-layer
which directly contacts the glow plug exchanges heat with the glow plug only by conduction. The sub-layer which directly connects to the left part of the gas cell (simply called the Left Gas Cell hereafter) transfers the heat to the left gas cell by heat conduction, and the convection term for the full size cell will be automatically taken care of by the original KIVA code itself by calculating the mass transfer term between the left gas cell and its neighboring full size cells.

3. Micro scale mass diffusion occurs between the sub-layers and the left gas cell. Although the gas stays quiescent at the macro scale, mass diffusion occurs between the sub-layers driven by the different concentration of each species. The governing law is Fick’s Law for mass diffusion.

4. The control volume method is used with fixed sub-layer boundaries and volumes. Because of the heat transfer, chemical reaction, and mass diffusion processes, each sub-layer will finally equilibrate to a new pressure common among the sub-layers and each sub-layer will reach its new mass and temperature value, with the mass re-distribution between the constant volume sub-layers.

The following section will present the mathematical model formulation that incorporates these assumptions.

6.3. Physical Models and General Forms of Differential Equations

![Figure 6.4 Illustration of infinitesimal sub-layer for differential form derivation.](image_url)
Within a thin cell near to the glow plug, several physical processes may occur simultaneously: chemical reaction, heat conduction, mass diffusion, and mass redistribution. We will analyze each physical process so as to set up a glow plug gas sub-layer model by discretization of a differential form of the governing equations. To facilitate this, we will analyze the property relationship between the infinitesimal distance from \( x = x \) to \( x = x + dx \) within a thin cell near to the glow plug, as shown in figure 6.4.

### 6.3.1. Chemical Reaction Model

A chemical reaction \( r \) is symbolized as:

\[
\sum a_{isp_r} \cdot \chi_{isp} = \sum b_{isp_r} \cdot \chi_{isp}
\]

where: \( isp \) is the index of species involved in the reaction \( r \);

\( \chi_{isp} \) represents one mole of species \( isp \);

\( a_{isp_r} \), \( b_{isp_r} \) are the integer stoichiometric coefficients for reaction \( r \).

The volumetric energy \( \dot{q} \) released from chemical reaction \( r \) is a function of local temperature (\( T \)), mass concentration of each species (density \( \rho \) and species fraction \( \chi \)):

\[
\dot{q}_r = Q_r \cdot \omega_r
\]

where: \( Q_r \) is the negative of the heat of reaction \( r \) at absolute zero,

\[
Q_r = \sum_{isp} (a_{isp_r} - b_{isp_r}) \cdot (\Delta h^0_j)_{isp}
\]
and \((\Delta h_f^0)_{isp}\) is the heat of formation of species \(isp\) at absolute zero*.

\(\omega_r\) is speed of the kinetic reaction \(r\),

\[
\dot{\omega}_r = k_{fr} \prod_{isp}(\frac{\rho_{isp}}{W_{isp}})^{a_{isp} \cdot \omega_r} - k_{br} \prod_{isp}(\frac{\rho_{isp}}{W_{isp}})^{b_{isp} \cdot \omega_r},
\]

where \(W_{isp}\) and \(\rho_{isp}\) are the molecular weight and density of the species \(isp\) involved in the reaction \(r\). Here \(\rho_{isp} = \rho \cdot X_{isp}\).

The exponents \(a_{isp \cdot \omega_r}\) and \(b_{isp \cdot \omega_r}\) specify the order of the reaction. \(a_{isp \cdot \omega_r}\) and \(b_{isp \cdot \omega_r}\) need not equal \(a_{isp \cdot \omega_r}\) and \(b_{isp \cdot \omega_r}\) so that empirical reaction orders can be used [Amsden, 1993].

The coefficients \(k_{fr}\) and \(k_{br}\) are the forward and backward rate coefficients for reaction \(r\) and are assumed to be of a generalized Arrhenius form:

\[
k_{fr} = A_{fr} \cdot T^{\zeta_{fr}} \cdot \exp\left(-\frac{E_{fr}}{T}\right), \text{ and }
\]

\[
k_{br} = A_{br} \cdot T^{\zeta_{br}} \cdot \exp\left(-\frac{E_{br}}{T}\right)
\]

where \(E_{fr}\) and \(E_{br}\) are activation temperatures (in Kelvin); \(A_{fr}, A_{br}, \zeta_{fr},\) and \(\zeta_{br}\) are the forward and backward coefficients.

So the volumetric energy release from all the chemical reactions is:

\[
\dot{q}_{chem} = \sum_r \dot{q}_r = \sum_r \left(\dot{Q}_r \cdot \dot{\omega}_r\right)
\]

Equation (6-4)

where: \(\dot{\omega}_r\) is a function of \((T, \rho, X)\), i.e.:

---

* Note that the thermodynamic properties built into KIVA are based on absolute zero.
\[
\dot{\omega}_r = \left( A_{fr} T^{\zeta_{fr}} \exp\left(-\frac{E_{fr}}{T}\right) \right) \prod_{isp} \left( \frac{\rho \cdot X_{isp}}{W_{isp}} \right)^{b_{isp \_r}} - \left( A_{br} T^{\zeta_{br}} \exp\left(-\frac{E_{br}}{T}\right) \right) \prod_{isp} \left( \frac{\rho \cdot X_{isp}}{W_{isp}} \right)^{b_{isp \_r}}
\]

Equation (6-5)

The mass change for each species due to the chemical reaction \( r \) is:

\[
\frac{\partial m_{r(isp)}}{\partial t} = W_{isp} \cdot (b_{isp \_r} - a_{isp \_r}) \cdot \omega_r \cdot (Adx)
\]

where \( A \) is the cross section area.

So the total mass change for each species due to all of the chemical reactions is:

\[
\frac{\partial m_{chem(isp)}}{\partial t} = \sum_r \left( \frac{\partial m_{r(isp)}}{\partial t} \right) = (Adx) \sum_r W_{isp} \cdot (b_{isp \_r} - a_{isp \_r}) \omega_r
\]

Equation (6-6)

The chemical kinetic mechanism used in this work is described in Appendix G.

6.3.2. Conductive Heat Transfer Model

There is only conductive heat transfer occurring within the thin gas cell without a convective heat transfer term. The net energy transferred into the slice between \( x \) and \( x+dx \) is governed by Fourier’s Law:

\[
\frac{\partial Q}{\partial t} = A \left( \frac{\partial q''}{\partial x} \right) dx
\]

where: \( q'' \) is the heat flux, \( q'' = k \left( \frac{\partial T}{\partial x} \right) \), \( k \) is the gas thermal conductivity. \( k \) is a function of temperature.
So, \[
\frac{\partial Q}{\partial t} = A \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) dx
\] 

Equation (6-7)

The thermal conductivity \( k \) is a function of temperature, and depends on \( x \), so it cannot be simply treated as a constant and taken out of the derivative.

The following boundary conditions discussed are independent and applied only within the glow plug model. The glow plug model then will interact with the KIVA main code for exchanging mass and energy, the flow chart of glow plug model implementation into KIVA code is shown in figure 6.9.

The boundary conditions for heat conduction are:

\( q=0 \) at \( x=0 \)

No heat conduction out of the gas cell. The heat transfer between the gas cell and its neighboring cells will be taken care of by the original KIVA code.

\( T=T_{gp} \) at \( x=x_{gp} \)

The wall temperature is given as \( T_{gp} \), which will be also computed by the glow plug model.

6.3.3. Mass Diffusion Model

The mass diffusion is driven by the mass fraction gradient of each species between the different sub-layers. It is governed by Fick’s Law, which can be expressed as:

\[
J_{(isp)} = -D_{isp} \cdot \rho \cdot \frac{dX_{(isp)}}{dx}
\]
where: \( J_{isp} \) is the mass diffusion flux for species \( isp \), in unit of \( \text{kg/m}^2\cdot\text{s} \).

\( D_{isp} \) is the mass diffusion coefficient for species \( isp \), also called the mass diffusivity, in unit of \( \text{m}^2/\text{s} \).

\( \rho \) is the density of the gases, in the unit of \( \text{kg/m}^3 \).

\( X_{isp} \) is the mass fraction for species \( isp \). \( X_{isp} \) is in the range of \( 0 \sim 1.0 \).

\( dX_{isp}/dx \) is the mass fraction gradient.

So the mass change for each species \( isp \) due to the mass diffusion is:

\[
\frac{\partial m_{\text{diff},isp}}{\partial t} = -A \left( \frac{\partial J_{isp}}{\partial x} \right) dx = A \frac{\partial}{\partial x} \left( D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) dx
\]

The energy change associated with mass diffusing across a system boundary is:

\[
\frac{\partial E_{\text{diff},isp}}{\partial t} = \frac{\partial (h_{isp} \cdot m_{\text{diff},isp})}{\partial t} = A \frac{\partial}{\partial x} \left( h_{isp} \cdot D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) dx
\]

The total mass change for all species due to the mass diffusion is:

\[
\frac{\partial m_{\text{diff}}}{\partial t} = \sum_{isp} \left( \frac{\partial m_{\text{diff},isp}}{\partial t} \right) = A \cdot dx \cdot \sum_{isp} \left[ \frac{\partial}{\partial x} \left( D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) \right]
\]  
Equation (6-8)

The total energy change associated with the mass diffusion for all species is:

\[
\frac{\partial E_{\text{diff}}}{\partial t} = \sum_{isp} \left( \frac{\partial E_{\text{diff},isp}}{\partial t} \right) = A \cdot dx \cdot \sum_{isp} \left[ \frac{\partial}{\partial x} \left( h_{isp} \cdot D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) \right]
\]  
Equation (6-9)

where: \( h_{isp} \) is the specific enthalpy for species \( isp \), \( h_{isp} = u_{isp} + P v_{isp} = c_{p,isp} T \), and

\( v_{isp} = 1/\rho_{isp} = 1/(\rho X_{isp}) \).

Boundary conditions for mass diffusion:
There is no mass diffusion out of the cell. The cell will interact with neighboring cells only by convection, which is considered by the original KIVA code. Also, there is no mass diffusion at the solid glow plug boundary.

6.4. General Forms of Governing Equations

6.4.1. Ideal Gas Equation

\[ PV = RmT, \text{ or } P / \rho = RT \quad \text{Equation (6-10)} \]

6.4.2. Mass Conservation Equation

The mass change of each species due to chemical reactions and mass diffusion is:

\[
\frac{\partial m_{(ip)}}{\partial t} = \frac{\partial m_{\text{chem}(ip)}}{\partial t} + \frac{\partial m_{\text{diff}(ip)}}{\partial t}
\]

\[
= (Adx) \sum_r \left[ W_{(ip)} \cdot (b_{r(ip)} - a_{r(ip)}) \cdot \dot{\omega}_r \right] + A \cdot \frac{\partial}{\partial x} \left[ D_{(ip)} \cdot \rho \cdot \frac{\partial X_{(ip)}}{\partial x} \right] \cdot dx
\]

Because:

\[
\frac{\partial m_{(ip)}}{\partial t} = \frac{\partial (\rho Adx X_{(ip)})}{\partial t}, \text{ so}
\]

\[
\frac{\partial (\rho X_{(ip)})}{\partial t} = \frac{\partial}{\partial x} \left( D_{(ip)} \cdot \rho \cdot \frac{\partial X_{(ip)}}{\partial x} \right) + \sum_r \left[ W_{(ip)} \cdot (b_{r(ip)} - a_{r(ip)}) \cdot \dot{\omega}_r \right] \quad \text{Equation (6-11)}
\]
6.4.3. Energy Conservation Equation

For energy conservation by chemical reaction, heat conduction, and mass transportation:

\[
\frac{\partial E}{\partial t} = \frac{\partial Q}{\partial t} + q_{\text{chem}} A dx + \frac{\partial E_{\text{diff}}}{\partial t}
\]

where: \( E \) is the internal energy in the differential element within \( x \) to \( x+dx \). \( E = (\rho Adx)(c, T) \)

Substitute each term with their expressions:

\[
\frac{\partial (\rho Adx c, T)}{\partial t} = A \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) dx + \sum_r \left( Adx q_r \right) + A \cdot dx \cdot \sum_{isp} \left[ \frac{\partial}{\partial x} \left( h_{isp} \cdot D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) \right]
\]

So, by simplification:

\[
\frac{\partial (\rho c, T)}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \sum_r \left( Q_r \omega_r \right) + \sum_{isp} \left[ \frac{\partial}{\partial x} \left( h_{isp} \cdot D_{isp} \cdot \rho \cdot \frac{\partial X_{isp}}{\partial x} \right) \right]
\]

Equation (6-12)

where: \( \omega_r \) is a function of \( (T, \rho, X) \) as indicated in equation (6-5).

6.5. Discretization of the Differential Forms

Now we need to discretize the thin gas cell into \( n \) sub-layers \( (i=1, \ldots, n) \) and one left gas cell \( (i=0) \). Let \( \Delta l_i \) be the thickness of sub-layer \( i \). For easy setup of the control volume method, we use an even thickness for all the sub-layers, i.e.,

\[
\Delta l_1 = \Delta l_2 = \cdots = \Delta l_i = \cdots = \Delta l_n = \Delta l
\]
The total volume of the thin gas cell is $V$, so the thickness of the left gas cell is:

$$
\Delta l_0 = \frac{V}{A} - \sum_{i=1}^{n} \Delta l_i.
$$

At time $t=t$, the pressure is equilibrated within the cell, i.e.

$$
P_0 = P_1 = P_2 = \cdots = P_i = \cdots = P_n = P.
$$

The same notation used with $P$ and $\Delta l$ will be applied to other properties, as illustrated in figure 6.5.

For simplicity in further illustrations, if it is not specified, the term of “sub-layers” includes both the left gas cell and the n-sub-layers, i.e. $i=0, 1, \ldots, n$.

![Diagram of discretized sub-layer system for the thin gas cell near glow plug.](image)

Figure 6.5 Illustration of discretized sub-layer system for the thin gas cell near glow plug. Note: $n$ is chosen to be 4 in the program.

At time $t=t+\Delta t$, after the chemical reaction, heat conduction, and mass diffusion, the pressure for each sub-layer is changed to $P_i'$, and the temperature is changed to $T_i'$, density changed to $\rho_i'$, and the mass fraction for each species changed to $X_{isp}'$. Now we can discretize the
differential form of the ideal gas equation, the mass conservation equation, and the energy conservation equation to derive their discretization form, as shown in figure 6.6.

![Diagram](image)

Figure 6.6 Illustration of the control volume method for mass and energy change for an individual sub-layer by chemical reaction, heat conduction, and mass diffusion processes

6.5.1. Discretized Form of the Ideal Gas Equation

\[ P_i V_i = R_i m_i T_i, \text{ or } \frac{P_i}{\rho_i} = R_i T_i \]

At time \( t=t \), as \( P_0 = P_1 = P_2 = \cdots = P_i = \cdots = P_n = P \), so

\[ \frac{P}{\rho_i} = R_i T_i \]

At time \( t=t+\Delta t \),

\[ \frac{P_i'}{\rho_i'} = R_i T_i' \]

Equation (6-13)
6.5.2. Discretized Form of Mass Conservation Equation

The equation (6-11) for mass conservation for each species $isp$ due to both mass diffusion and chemical reactions can be written into the discretized form as:

$$\frac{\rho_i X'_i - \rho_i X_i}{\Delta t} = \frac{D_{isp}}{\Delta l} \left[ \left( \rho_{i/i+1} \cdot \frac{X_{i+1} - X_i}{\Delta l} \right) - \left( \rho_{i-1/i} \cdot \frac{X_i - X_{i-1}}{\Delta l} \right) \right]$$

$$+ \sum_r \left[ W_{isp} \cdot (b_{r(iup)} - a_{r(iup)}) \cdot \omega_r \right]$$

It can be simplified as:

$$\frac{\rho_i X'_i - \rho_i X_i}{\Delta t} = \frac{D_{isp}}{\Delta l^2} \left[ \rho_{i/i+1} \left( X_{i+1} - X_i \right) - \rho_{i-1/i} \left( X_i - X_{i-1} \right) \right]$$

$$+ \sum_r \left[ W_{isp} \cdot (b_{r(iup)} - a_{r(iup)}) \cdot \omega_r \right]$$  \hspace{1cm} \text{Equation (6-14)}

where: $\rho_{i/i+1}$ is the density at the boundary between sub-layer $i$ and sub-layer $i+1$.

$$\rho_{i/i+1} = (\rho_i + \rho_{i+1})/2$$

$\cdot \omega_r$ is chemical reaction speed for reaction $r$ in sub-layer $i$. In discretized form, $\cdot \omega_r$ can be expressed as a function of $(T_i, \rho_i, X_{i(isp)})$:

$$\cdot \omega_r = \left( A_p T_i \exp \left( - \frac{E_f}{T_i} \right) \right) \prod_{isp} \left( \frac{\rho_i \cdot X_{i(isp)}}{W_m} \right) \cdot \omega_r - \left( A_h T_i \exp \left( - \frac{E_h}{T_i} \right) \right) \prod_{isp} \left( \frac{\rho_i \cdot X_{i(isp)}}{W_m} \right) \cdot h_r$$  \hspace{1cm} \text{Equation (6-15)}
Consider the boundary conditions:

For the left gas cell, i.e. at $i=0$,

$$\frac{(\rho'_{0}X'_{0(isp)}) - \rho_{0}X_{0(isp)})}{\Delta t} = \frac{D_{isp}}{\Delta l^2} \left[ \rho_{0/(i)} \left( X_{1(isp)} - X_{0(isp)} \right) - 0 \right] + \sum_{r} \left[ W_{isp} \cdot (b_{r(isp)} - a_{r(isp)}) \omega_{r} \right]$$

For the last sub-layer nearest to the glow plug, i.e. at $i=n$,

$$\frac{(\rho'_{n}X'_{n(isp)}) - \rho_{n}X_{n(isp)})}{\Delta t} = \frac{D_{isp}}{\Delta l^2} \left[ 0 - \rho_{n-1/(i)} \left( X_{n(isp)} - X_{n-1(isp)} \right) \right] + \sum_{r} \left[ W_{isp} \cdot (b_{r(isp)} - a_{r(isp)}) \omega_{r} \right]$$

Taking the summation of equation (6-14) for all species of $isp$, at both sides of the equation, we have:

$$\sum_{isp} \frac{(\rho'_{i}X'_{i(isp)}) - \rho_{i}X_{i(isp)})}{\Delta t} = \frac{(\rho'_{i} - \rho_{i})}{\Delta t}$$

$$= \sum_{isp} \left[ \frac{D_{isp}}{\Delta l^2} \left[ \rho_{i+1/(i)} \left( X_{i+1(isp)} - X_{i(isp)} \right) - \rho_{i-1/(i)} \left( X_{i(isp)} - X_{i-1(isp)} \right) \right] \right] + \sum_{isp} \left[ \sum_{r} \left[ W_{isp} \cdot (b_{r(isp)} - a_{r(isp)}) \omega_{r} \right] \right]$$

Equation (6-16)

From equation (6-16), the new density $\rho'_{i}$ for each sub-layer $i$ can be found, then for each individual species $isp$, $X'_{isp}$ can be found from equation (6-14).

6.5.3. Discretized Form of Energy Conservation Equation

The differential form of equation (6-12) for energy conservation by chemical reaction, heat conduction, and mass diffusion can be written into the discretized form as:
where: $h_{i/i+1(isp)} = c_{p_{-i/i+1(isp)}} \cdot T_{i/i+1}

k_{i/i+1}, h_{i/i+1(isp)}, c_{p_{-i/i+1(isp)}},$ and $T_{i/i+1}$ are the properties at the boundary between sub-layer $i$ and sub-layer $i+1$.

$$k_{i/i+1} = \frac{(k_i + k_{i+1})}{2}, \quad c_{p_{-i/i+1(isp)}} = \frac{(c_{p_{-i(isp)}} + c_{p_{-i+1(isp)}})}{2}, \quad T_{i/i+1} = \frac{(T_i + T_{i+1})}{2}$$

From equation (6-17), a new temperature $T_i'$ for each sub-layer $i$ can be found. Then, the new pressure $P_i'$ for each sub-layer can be found from the ideal gas equation (6-13). Thus all the other properties can be found.

### 6.6. Mass Re-distribution Process to Balance the Pressure

After the three processes of chemical reaction, heat conduction, and mass diffusion, the new energy and mass concentrations for each species do not equilibrate, thus generating pressure differences between each sub-layer. To reach the equilibrium, the mass within the sub-layers needs to be re-distributed, until the pressure reaches a balance in the whole thin gas cell,

i.e., $P_0'' = P_1'' = \ldots = P_i'' = \ldots = P_n''$
In sub-layer $i$, the mass re-distribution amount crossing the left side and right side are $\Delta m_i$ and $\Delta m_{i+1}$, associated with the energy transportation by $\Delta E_i$ and $\Delta E_{i+1}$, $(i=1,\ldots,n)$, as shown in figure 6.7. Setting the positive direction of the mass re-distribution to be from right to left, the following are the governing equations for sub-layer $i$ for the mass re-distribution process.

6.6.1. Ideal Gas Equation

\[
P_{i}^{''}/\rho_{i}^{''} = R_{i}^{''}T_{i}^{''}
\]

Equation (6-18)

6.6.2. Mass Conservation Equation

For sub-layer $i$,

\[
m_{i}^{'} = m_{i}^{'} + \Delta m_{i+1} - \Delta m_{i}
\]

(for overall mass) Equation (6-19)

\[
m_{i(isp)}^{'} = m_{i(isp)}^{'} + \Delta m_{i+1} \cdot X_{i+1/isp} - \Delta m_{i} \cdot X_{i/isp}
\]

(for each species isp) Equation (6-20)
where: $X'_{i;/i+1(isp)}$ is the fraction of the mass concentration of species $isp$ at the boundary of sub-layer $i$ and sub-layer $i+1$.

Boundary conditions:

For the left gas cell of $i=0$,

$$m^*_{0} = m^*_0 + \Delta m_i$$

$$m^*_{0(isp)} = m^*_0(isp) + \Delta m_i \cdot X'_{0;/1(isp)}$$

For the last sub-layer of $i=n$,

$$m^*_{n} = m^*_n - \Delta m_n$$

$$m^*_{n(isp)} = m^*_n(isp) - \Delta m_n \cdot X'_{n-1;/n(isp)}$$

### 6.6.3. Energy Conservation Equation

For sub-layer $i$,

$$E^*_i = E'_{i} + \Delta m_{i+1} \cdot h'_{i;/i+1} - \Delta m_i h_{i-1;/i}$$  \hspace{1cm} \text{Equation (6-21)}$$

where: $X'_{i;/i+1(isp)}$ is the fraction of the mass concentration of species $isp$ at the boundary of sub-layer $i$ and sub-layer $i+1$.

$h'_{i;/i+1}$ is the specific enthalpy at the boundary of sub-layer $i$ and sub-layer $i+1$.

Because: $E_i = c_{pi} \cdot m_i \cdot T_i = \frac{c_{pi}}{R_i} \cdot P_i \cdot V_i = \frac{P_i \cdot V_i}{\gamma_i - 1}$, the energy conservation equation can be re-written as:
\[ \frac{P_i^* \cdot V_i}{(\gamma_i^* - 1)} = c_{\text{v}i} \cdot m_i^* \cdot T_i^* + \Delta m_{i+1} \cdot h_{i/i+1} - \Delta m_i h_{i-1/i} \] \hspace{1cm} \text{Equation (6-22)}

Boundary conditions:

For the left gas cell of \( i=0 \),

\[ \frac{P_{0}^* \cdot V_0}{(\gamma_0^* - 1)} = c_{\text{v}0} \cdot m_0^* \cdot T_0^* + \Delta m_1 \cdot h_{0/1} \]

For the last sub-layer of \( i=n \),

\[ \frac{P_n^* \cdot V_n}{(\gamma_n^* - 1)} = c_{\text{v}n} \cdot m_n^* \cdot T_n^* - \Delta m_n h_{n-1/n} \]

6.6.4. Mathematical Approach of Solving the Mass Re-distribution Process

From the set of energy conservation equations (6-22), the total number of the equations is \( n+1 \). The ratio of specific heats \( \gamma \) can be treated as a function of \( x \) only (different temperatures at different locations), but will not change within a small time step for the small amount of mass re-distribution, so \( \gamma_i^* \) can be replaced by a known property of \( \gamma_i^* \). Then the total number of unknowns is also \( n+1 \), i.e., \( P_i^* \), and \( \Delta m_i \ (i=1,\ldots,n) \), which can be found by solving a set of linear equations.

After this, from the mass conservation equations (6-19) and (6-20), \( m_i^{\text{up}} \) and \( m_i^* \) can be found. Then from ideal gas equation (6-18), \( T_i^* \) can be found, thus all the other properties can be found as well.
Based on these discretized governing equations, a novel gas sub-layer model was developed, which includes sub-models of chemical reaction, heat conduction, mass diffusion, and mass re-distribution. It uses the implicit method to solve the discretized equations. Thus, the time step was kept the same as the KIVA-3V optimized value without further restrictions. To increase the accuracy, the interpolation of gas properties was changed from two-point interpolation in the original KIVA code to three-point interpolation.

6.7. Physical Processes of the Glow Plug Ignition Model and Its Incorporation with KIVA Main Code

This virtual gas sub-layer model was used with the glow plug discretized model described in chapter 5 together as a glow plug ignition model to study the physics of the glow plug ignition process. After the development of this glow plug ignition model, it needs to be incorporated with the KIVA main code so as to simulate the glow plug ignition process. This section summarizes the physical processes for the glow plug ignition model, and details the heat and mass transfer situations. Some of these physical processes provide the links between the glow plug ignition model and KIVA main code.

6.7.1. Heat Conduction within the Glow Plug Discretized Cells

The glow plug is discretized into small cells and conducts the heat from inner layers to outer layers when the glow plug surface has a lower temperature, e.g., at the time of heating up the surrounding gas. There is an internal heat source term applied at the inside boundary layer. This conductive heat transfer is determined by the glow plug discretised model.
When the glow plug surface has a higher temperature, e.g. after the ignition when the outer surface is heated by hot combustion products, the conductive heat transfer direction is from outer layers to inner layers.

6.7.2. Heat Transfer between the Surface of the Glow Plug and the Adjacent Virtual Gas Sub-layers

The glow plug discretized model only internally interacts with the virtual gas sub-layer model inside the glow plug ignition mode. The heat transfer is between the solid glow plug surface cells and their adjacent virtual gas sub-layers.

Since the local surrounding gas temperature can be very different, the transient heat transfer between the glow plug surface cells and the adjacent virtual gas sub-layers becomes very different too, such as during the strong cooling when the natural gas jet is impinging onto the glow plug surface, or strong local heating occurs near the ignition spot after ignition is initiated. Thus the glow plug may have transient temperature variations over the different surface locations as well as through the different thickness of glow plug layers.

6.7.3. Heat Transfer and Thermal Boundary Layer Formation within the Adjacent Virtual Gas Sub-layers

At the time of the beginning of the computation and before the fuel jet reaches the glow plug, the glow plug surface has a much higher temperature than the surrounding gas, and releases heat to the adjacent virtual gas sub-layers. Thus the virtual gas sub-layers are heated and form a thin thermal boundary layer within them, which is on the micrometer scale. The convective heat transfer is neglected within the virtual gas sub-layers, so only heat conduction will be considered.
by the virtual gas sub-layer model. Figure 6.8 shows the thermal boundary layer development within the virtual gas sub-layers from simulation result of the glow plug model.

From the figure, it can be seen that within the short time (100 µs) before fuel jet reaches the glow plug, the thermal boundary layer is very thin with a high temperature gradient within this thermal boundary layer. The growth and development of the thermal boundary layer is similar to the analytical result shown in figure 6.1.

![Figure 6.8](image)

Figure 6.8 Thermal boundary layer development. 4 virtual gas sub-layers were chosen, gas initial temperature was 900 K, glow plug initial surface temperature was 1300 K.

6.7.4. Fuel Diffused into the Virtual Gas Sub-layers after Reaching Glow Plug

When the fuel jet arrives the thin gas cells adjacent to the glow plug surface which contain the virtual gas sub-layers, the fuel is diffused into the virtual gas sub-layers by mass diffusion model within the virtual gas sub-layer model.
6.7.5. Physical Processes within the Virtual Gas Sub-layers

After the fuel is diffused into the virtual gas sub-layers, the chemical reaction speeds are very different within these virtual sub-layers since they have a high temperature gradient located in the thermal boundary layer. Thus the temperature and the mass concentration of each species become very different between each virtual gas sub-layers. Heat conduction takes place between the virtual gas sub-layers and the left gas cell by the heat transfer model. The species of chemical reaction products are transported out of the virtual gas sub-layers into the left gas cell in the same thin gas cell by mass diffusion model. At the same time, energy also will be transported with this mass transfer. As a result, the left gas cell consumes fuel and generates chemical reaction products, and the temperature in the left gas cell increases. These processes are all taken care of by the virtual gas sub-layer model.

6.7.6. The Link – Consideration of Left Gas Cell in KIVA main Code

The new properties of the left gas cell with high temperature and high concentration of chemical reaction products are then being sent back to the KIVA main code, so that the mass and energy exchange with its neighbored cells can be taken care of by the KIVA main code with conventional CFD convective governing equations. The interaction and incorporation of the glow plug model with KIVA main code is as shown in the program flow chart in figure 6.9. As a result, the products can be carried away from the left gas cell, and new fuel supplied into the left gas cell. The heat generated from the chemical reactions within the virtual gas sub-layers is transported outside of the cell into its neighbor cells.
6.7.7. Re-consideration of Left Gas Cell in Virtual Gas Sub-layer Model – Mass Redistribution Model

After the left gas cell interacts with its neighbor gas cells by KIVA code, the new updated properties are being input back into the virtual gas sub-layer model. The mass re-distribution model balances the pressure between the left gas cell and the virtual sub-layers. Then the next iteration of the glow plug ignition model will be performed.
As a result, if the local convection around the glow plug is too high, heat can not be accumulated in the left gas cell and its neighboring cells, and ignition will not happen in this region. But at some locations where the flammable fuel air mixture continues to be supplied to the left gas cell and convective heat loss is at proper level, e.g., at the back of the glow plug in the jet attachment region, there is a positive net heat transfer into the left gas cell, the left gas cell temperature may keep on increasing, and finally reaches local ignition temperature in this region. The detailed ignition location will be introduced in chapter 7 from the simulation results generated by this glow plug ignition model.

In summary, the glow plug discretized model and the virtual gas sub-layer model reveal the physics of the ignition process including transient heat transfer, chemical reaction, and mass diffusion within micrometer thin layers. In the following chapter, the glow plug ignition model will be applied for several case studies on the natural gas ignition and combustion, and the ignition simulation result will be discussed.
Chapter 7

Results of Simulation for the Natural Gas Ignition

The solid glow plug discretized model and the gas sub-layer model were developed to work together to simulate the glow plug assisted natural gas ignition process.

This chapter presents the simulation results for methane ignition by a bare glow plug, as well as by a shielded glow plug, and compares the simulation results against the experimental results. Results are also presented for studies of some combustion situations such as multi-pulse injection and the leakage of fuel from the injector.

For methane, the main component of natural gas, KIVA-3V has two built-in models for its combustion. The first is a one-step kinetic reaction model with first moment closure for the chemical source terms. The second is turbulence mixing controlled chemistry model, where a mixing dominates the chemical reaction rate during diffusion combustion, based on assuming that the kinetic chemical reaction rate is infinitely faster than the physical turbulence mixing rate.
However, KIVA-3V does not have appropriate conditions for when to use these models. Micklow and Gong [2001] studied the conditions for effectiveness of the chemical control and physical control rates. The details are introduced in Appendix G.1.

Compared to higher-level closure models such as second moment closure or conditional moment closure, first moment closure for the chemical source term under turbulence condition is not accurate enough unless the chemical reaction rates are well tuned against experimental results, especially if the focus is on the ignition stage only, (one of the main objectives for this research is to develop a model for glow plug ignition rather than the further combustion and emission). The details for turning for the chemical reaction rates are introduced in appendix G.2.

The glow plug ignition model will work better with improvements to the chemical reaction models such as improvement from one-step to multi-step models (e.g. two-step model), although the computational load needs to be taken into consideration. The details of these improvements are recommended in chapter 9.

Simulations were conducted using the solid glow plug discretized model and the gas sub-layer model to investigate four aspects of natural gas ignition, namely: simulation of natural gas ignition over a bare glow plug, simulation of natural gas ignition over a shielded glow plug, simulation of multi-pulse injection and ignition, and simulation of leakage from the injector nozzle after pintle shut off.
7.1. Simulation of Natural Gas Ignition Over a Bare Glow Plug

For the case of simulating ignition over the bare glow plug, in order to improve the grid density near the glow plug to allow a more significant temperature gradient, a second thin gas layer was added to the thin gas layer which is contacting the glow plug as comparison to only one thin gas layer as shown in figure 6.2. The grid structure of the two gas layers is shown in figure 7.1. The two layer structure is used in all ignition simulations presented in this chapter.

Figure 7.1 Structure of the grid for two thin gas layers surrounding the glow plug. Left: overall grid structure; Right: detail view of two thin gas layers surrounding the glow plug.

7.1.1. Simulation of Fabbronni’s Experiments at Low Bulk Gas Temperature

Fabbronni [2004] did many experiments on single jet injection (gas supply conditions of 11MPa and 400K) into the combustion chamber (air at 899K and 4.9 MPa) for different injection durations varying from 1 ms to 8 ms using a bare glow plug. His experimental results show that the ignition occurs in less than 2 ms with an average of 1.75 ms, no matter what injection duration is used.
Simulations of Fabbroni’s experiments were conducted for the case of combustion chamber air temperature of 899 K and pressure of 4.9 MPa at TDC. The injection upstream condition was 400 K and 11 MPa, and the nozzle diameter was 0.344 mm. The glow plug was placed 15° upstream of the nozzle center line, where upstream refers to the swirl direction.

As introduced in section 4.5.4, poppet valve model was compared to the velocity boundary condition and pressure boundary condition applied on the same above mentioned experimental conditions for the ignition simulation. The simulation results showed that the poppet valve model has an ignition delay time of 1.76 ms and agrees better with the experiment result compared to 1.41 and 1.40 ms ignition delay time from the velocity and pressure boundary conditions. All the following simulations in this chapter then use the poppet valve model working together with glow plug ignition model for the ignition and combustion study.

For a typical injection duration of 2 ms, the ignition delay with the poppet valve model was calculated to be 1.76 ms. Figure 7.2 shows the calculated temperature and fuel-air equivalence ratio in the plane of the nozzle centerline just after ignition at 1.76 ms.

The figures present a two-dimensional representation of temperature and fuel-air equivalence ratio in the three-dimensional fuel jet structure. A stoichiometric mixture of methane and air has a fuel-air equivalence ratio \( \phi \) of 1.0. A methane-air mixture is flammable over the range \( \phi = 0.5 \) (lean) to \( \phi = 1.5 \) (rich). Mixtures with fuel-air equivalence ratios less than 0.5 or greater than 1.5 are too lean or too rich respectively to sustain flame propagation.
Figure 7.2 shows that the largest flammable mixture region is on the back (relative to the injector nozzle) of the glow plug in the flow attachment region. Using an ignition criterion of $T = 2000$ K, figure 7.2 (left) shows that the ignition position was also at the back of the glow plug in the flow attachment region where flammable mixture has the longest residence time exposed to heat transfer from the hot glow plug which was discussed in previous section 4.4.3.

The velocity profile around the flow plug in figure 7.3 clearly shows that air is entrained into the methane jet at both the front and the back of the glow plug to form the fuel air mixture, and two stagnation positions are found in these two regions. However, compared to the back attachment region, the front one experiences a direct impingement of the cold jet with a thinner flammable region, so the ignition does not start in the front region, but at the back one.
This computed result is consistent with the ignition position identified in the experiments conducted by Abate [2001] at similar conditions. The nozzle centerline in the pictures from the experiments is rotated counterclockwise roughly 45 degrees compared to the simulations, but figure 7.4 shows ignition at the back of the glow plug. Note the injector nozzle position marked in frame 6 of the ignition sequence captured with an ICCD camera. This ability to compute the correct ignition position gives some confidence in the accuracy of the glow plug ignition model.
Simulations were carried out at several different injection durations. The ignition delay values calculated by the simulation are listed in table 7-1. The simulation results confirm the experimental results that, for injection durations longer than 2 ms, the ignition delay was constant at 1.7 ms regardless of the injection duration.

Table 7-1 Simulation results of ignition delay at different injection durations.

<table>
<thead>
<tr>
<th>Injection duration (ms)</th>
<th>1.0</th>
<th>2.0</th>
<th>4.0</th>
<th>7.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ignition delay (ms)</td>
<td>1.0</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7</td>
</tr>
</tbody>
</table>

However, the situation is different at injection durations shorter than 2.0 ms. At an injection duration of 1.0 ms, the ignition delay was only 1.0 ms compared to 1.7 ms for injection durations more than 2 ms. This is because of the pintle lift profile, shown in figure 7.5.
As shown in figure 7.5, a feature of the injector pintle lift is fast opening (within 0.1 ms) and slow closing (within 0.5 ms) response. The difference in the rate of injector opening and closing speeds is due to the injection design. The different opening and closing speeds have some impact on the ignition and combustion process.

For the case of 2 ms injection duration, the jet reaches the glow plug at about 0.1 ms, and continues at full momentum until the injector begins to close at about 1.5 ms. During this period the convection cooling effect of the cold gas jet on the bare glow plug is enormous. Thus, much of the heat released from chemical reaction in the high-temperature gas sub-layers near the glow plug is convected away by the flow of the cold jet. However, as long as enough heat accumulates and the temperature reaches ignition (criterion is 2000 K) in local gas cells (not sub-layers), it does not matter if the injection duration is more than 2 ms, the ignition occurs anyway.

For the case of 1 ms injection, since the mixed air-gas sub-layers near the glow plug accumulate heat from 0.1 ms, when gas first reaches the glow plug. At 0.5 ms, the pintle starts to close, and gradually cuts off the methane injection. So the jet slows down after 0.5 ms, the convective heat loss due to the cold jet flow decreases, and heat can be accumulated much faster.
The net result is to make the ignition occur faster than it does with the 2 ms and longer injection durations.

Achieving a shorter ignition delay with a shorter injection duration suggests an interesting possibility of multi-pulse natural gas injection, combining a first short injection pulse to achieve quick ignition, followed by a long injection afterwards. This technique is already used in some diesel engines. This new idea for natural gas injection was simulated and will be discussed later in section 7.4.

7.1.2. Simulation of Abate’s Experiments at High Bulk Gas Temperature

Abate [2001] conducted some experiments on bare glow plug ignition under conditions of higher temperature for the bulk gas (1242 K and 4.4 MPa). The ignition delay from his experiments was 0.45 ms, much shorter than might be expected for the higher temperature.

A simulation was performed for the same conditions as this experiment and the ignition delay calculated by the simulation was 0.42 ms. This is good agreement with the experimental data.

These two simulations, one at low bulk gas temperature and one at high bulk gas temperature, show that the solid glow plug discretized model together with the gas sub-layer model works well to simulate ignition over a bare glow plug for natural gas fuel injection.
7.2. Independence Study of Mesh Density for Natural Gas Ignition

To study the mesh density independence for natural gas ignition, simulations of a single jet under Fabbroni’s experimental condition with 2 ms injection duration were performed on three different mesh densities: a course mesh, a regular mesh, and a fine mesh. These are the same three mesh densities used for the grid independence study of jet simulation (without the glow plug) previously described in section 4.3 (see table 4-2).

The detailed structures of the three meshes are shown in figure 7.6.

![Figure 7.6 The structure of coarse, regular, and fine mesh with 2 thin gas layers surrounding the glow plug.](image)

The ignition delays calculated using these 3 mesh structures are shown in table 7.2. From the table, it can be seen that the coarse mesh has a large difference (37.5%) compared to the fine mesh, since the restriction of two thin gas layers not only makes the mesh at the back of the glow plug extremely large (only 3 layers available) but also distorts the shape of the mesh at the front of the glow plug. This distortion makes the point of ignition much offset compared to the one with the fine mesh. The regular mesh size significantly improved the mesh structure compared to the coarse mesh, and is very similar to the structure of the fine mesh. Use of the regular mesh
reduced the difference in ignition delay to 6.3% compared to the fine mesh. Although this is still a relatively large difference, the regular mesh shows the convergence trend with an affordable computational load. So, the regular mesh structure was applied to the subsequent ignition studies.

Table 7.2 Comparison of simulation results for ignition delay.

<table>
<thead>
<tr>
<th>Mesh structure</th>
<th>Coarse mesh</th>
<th>Regular mesh</th>
<th>Fine mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ignition delay (ms)</td>
<td>1.0</td>
<td>1.7</td>
<td>1.6</td>
</tr>
<tr>
<td>Difference</td>
<td>37.5%</td>
<td>6.3%</td>
<td>--</td>
</tr>
</tbody>
</table>

7.3. Simulation of Natural Gas Ignition Over a Shielded Glow Plug

As introduced in section 4.4.3, a round shield has been added surrounding the glow plug with an opening turned toward the jet. The advantages of having a shield surrounding the glow plug were explained in section 4.4.3 and the structure of the shielded glow plug was shown in figure 4.15.

Simulations of methane ignition for the shielded glow plug case were performed. In the combustion bomb, the initial bulk air temperature was 850 K and the pressure was 4 MPa. The injection supply pressure was 11 MPa, the temperature was 400 K, and the injection duration was 4 ms. The simulations showed that ignition started 1.65 ms after injection. Fabbroni [2004] conducted experiments at these conditions and measured an average of 1.55 ms ignition delay for the shielded glow plug. The simulation results agree very well with the experimental results. Figure 7.7 shows the calculated temperature profile and fuel air equivalence ratio profile at 1.7 ms with the shielded glow plug.
Figure 7.7 shows that the ignition location (T > 2000 K) was at the front flammable region attached to the glow plug, which agreed with the expected ignition location discussed in section 4.3.4. The long residence time of this flammable region at the same place attached to the glow plug facilitates the chemical reactions that lead to ignition.

Under the same bulk air condition, the simulation shows that ignition cannot be initiated without the shield, using only the bare glow plug. From this, the benefit of the shield is clearly evident: it keeps the glow plug locally at high temperature by reducing the convective heat loss. At the same time, it increases the residence time of the flammable mixture adjacent to the glow plug. It is believed that a shielded glow plug may also make ignition more stable under different swirl conditions and injection durations, which represents different engine operation conditions.

Figure 7.8 shows the process of flame propagation outward through the slot in the shield and subsequent spread into the combustion chamber. Graphs of four separate parameters, temperature, fuel-air equivalence ratio, carbon monoxide concentration (CO), and carbon dioxide...
(CO\(_2\)) concentration, are shown at each time. Because of the one step chemical reaction mechanism, CO is one species of equilibrium reactions. Although CO is not a direct intermediate product of combustion, it still reflects the intensity of the chemical reaction speeds at high temperature, so carbon monoxide concentration can indicate the location of chemical reaction activity. As a combustion product, carbon dioxide concentration indicates where combustion is complete, especially at where the temperature drops down and CO concentration is low. All four parameters viewed together help to interpret the injected methane is ignited by the glow plug and subsequently burned.

From the figure it can be seen that from the time of 1.7 ms when the ignition started (local T>2000K), the flame took about 0.7 ms (until 2.4 ms after start of injection) to propagate outside of the shield. During this time, the flame first propagated inside the shield. This might be because in the mixture contained between the shield and the glow plug, the temperature was higher than that surrounding the cold jet core. As the flame spread inside the shield, the temperature became higher and the flame grew stronger. It then propagated outside the shield through the slot to the cold fuel jet. During this time, the fuel jet near the shield had been also heated to reach a higher temperature for the preparation of the flame propagation. The CO profile in figure 7.8 highlights the location of combustion regions of chemical reaction. The CO\(_2\) profile helps to illustrate the extent of combustion completeness when viewed together with the fuel-air equivalence ratio (which show the location of unburned fuel), and carbon monoxide (which shows regions currently reacting).

At times 7.7 ms and 10.0 ms, figure 7.8 shows that a little leakage of methane came out of the nozzle from the injector sac volume. The fate of this fuel will be discussed in section 7.5.
Figure 7.8 Ignition and flame propagation process for the shielded glow plug. The first row is the temperature profile, the second row is the fuel-air equivalence profile ($\phi=0\sim2$), the third row is the CO profile, the last row is the CO$_2$ profile.
7.4. Simulation of Multi-Pulse Injection and Ignition

Simulation results previously described in section 7.1.1 reveal that, when the injection duration was reduced from 2 ms to 1 ms, the ignition delay also decreased from 1.7 ms to 1.0 ms. The reduction in ignition delay generates an interesting opportunity to utilize multi-pulse injection for natural gas fueled engines, similar to the strategy employed in some modern diesel engines. This will not only shorten the ignition delay time, but more importantly, it may also decrease the pressure rise caused by large accumulation of fuel during the ignition delay period with a single long injection. The rate of pressure rise affects the engine mechanical and thermal loads as well as the noise generated. By replacing one long injection pulse with several short injection pulses, the jet penetration length is effectively reduced, limiting impingement of the fuel jet onto the cold combustion chamber wall, which has negative effects on combustion due to low temperatures and inadequate mixing.

Simulation was performed for the case of 2 injection pulses: a 1 ms initial pulse at the beginning and a 2 ms pulse afterwards with a 1 ms pintle shut-off period in between. The phasing of the valve lift is shown in figure 7.9.

![Figure 7.9 Phasing of two-pulse injection with a 1 ms shut-off period in-between.](image-url)
Figure 7.10 The process of two-pulse injection and ignition.

$t = 1.05$ ms

$t = 1.68$ ms

$t = 1.98$ ms

$t = 2.05$ ms

$t = 2.14$ ms

$t = 2.45$ ms

$t = 3.21$ ms
The simulation result of this two-pulse injection shows that as expected, following the first pulse injection, ignition started at about 1.0 ms, and then the flame propagated through the accumulated mixture. When the second pulse started to feed the new fuel jet into the chamber starting at 2 ms, the combustion of the fuel-air mixture from the first jet has become strong enough that the second cold jet did not quench it. The second fuel injection pulse was instead heated and ignited by the burning fuel from the first jet ignition. This ignition and flame propagation process is illustrated in figure 7.10.

Figure 7.10 presents temperature, fuel-air equivalence ratio, carbon monoxide concentration, and carbon dioxide concentration profiles at selected times after the start of the first injection. At time t=1.05 ms, when the injector valve has fully closed, ignition was initiated at the back of the glow plug. At time t=1.68 ms, a flame propagates from the ignition point but the jet was weaker since no more methane is arriving to feed the combustion. At time t=1.98 ms, near the end of the injector closed period, the first single jet is mostly combusted. At the next moment of t=2.05 ms, the second pulse is started, and it can be seen that new fuel was injected just outside of the nozzle. At time t=2.14 ms, combustion has become stronger, and most of the first jet was burned. At the same time the second injection formed a strong cold jet which was fed into the combustion zone. At time t=2.23 ms, the fuel from the first jet was all burned, and the second jet started to ignite. Because of the cold temperature of the second jet and the small flammable region at the second jet front due to relatively little oxygen entrained locally in the first jet combusted zone, the combustion was deteriorated, which is clearly shown from the weaker CO profile compared to the previous time of t=2.14 ms. Also the temperature decreased. At t=2.45 ms and t=3.21 ms, as the injection continued and the jet kept growing, intense combustion resumed as can be deduced from the temperature and CO profiles.
From the process, it can be seen that the important factor affecting the success of the second fuel jet pulse ignition is the shut-off time of the injection between two pulses. If it is too short, before flame propagation from the first jet ignition point is well established, the flame may be quenched. If the second injection starts too long after the main combustion finishes for the first jet, it may not be ignited at all by the late weak combustion of the first jet.

7.5 Simulation of Leakage from The Injector Nozzle after Pintle Shut Off

Leakage of fuel gas from the nozzle after the injector shut-off is the one of the main sources for unburned hydrocarbon emissions. There is a finite volume in the injector nozzles downstream of the pintle and seat. As the pressure in the cylinder falls during the expansion process, fuel gas stored in this injector volume expands out into the combustion chamber. This “leakage” has low momentum and therefore doesn’t mix well. Consequently, it may not be burned but is instead exhausted as hydrocarbon (HC) emissions.

Simulation was performed to study the leakage characteristics, including when the leakage happens, whether part of the fuel from the leakage can be burned, when the leakage stops, etc. To save computational time, a 1 ms short injection duration was chosen for the simulation. The simulation conditions are: methane injection pressure of 11 MPa and temperature of 400 K, a combustion chamber pressure of 4.9 MPa and temperature of 899 K with a glow plug initial temperature of 1400 K.

Figure 7.11 shows the history of average pressure and maximum temperature in the combustion chamber, as well as the average pressure in the injector. Figure 7.12 shows the fuel air equivalence ratio profile at several different times, which illustrates the methane content in the combustion chamber. Note that to adequately show the extent of fuel mixing and dispersion,
the range of the fuel air equivalence ratio was chosen to be 0~2.0 instead of the flammable range of 0.5~1.5 as was used before. Figure 7.13 shows the velocity direction within the nozzle at different times.

Figure 7.11 The computed time history of average pressure of injector and combustion chamber and the maximum temperature in the combustion chamber.

Figure 7.12 The temperature profile and fuel air equivalence ratio profile in the combustion chamber at different times before and after the end of injection.

(1) $t=1.9\text{ms}$  (2) $t=2.1\text{ms}$  (3) $t=2.4\text{ms}$  (4) $t=2.7\text{ms}$  (5) $t=3.2\text{ms}$  (6) $t=6.3\text{ms}$
Figure 7.13  Velocity direction of the methane inside the fuel injector nozzle at different times.

From figure 7.11, it can be seen that after the injector shut off at 1.0ms, methane kept injecting out into the combustion chamber from the injector as the pressure in the injector decreased. Because combustion occurred in the combustion chamber, the pressure and temperature in the combustion chamber increased. At about 1.9 ms, the pressure in the injector dropped to the same value as in the combustion chamber. However, because of the fuel jet momentum, the methane was still being injected out into the combustion chamber, as shown in figure 7.12-(1) and 7.13-(1). After t = 1.9 ms, the pressure in the combustion chamber is higher than the pressure in the injector, so the injection velocity was decreased. At about t=2.1 ms, the pressure in the combustion chamber had already pushed the methane back from the nozzle into the injector. The fuel jet velocity in the backward direction is shown in figure 7.13-(2). At this point the jet was cut off from the nozzle. At t=2.4 ms, most of the front of the jet had burned with only the jet tail remaining. The remaining fuel was blown offset from the nozzle by the swirl as shown in figure 7.12-(3). Also at this time, since much of the jet had been combusted, the temperature started to drop from the peak value. At t = 2.7 ms, the jet had almost all burnt as shown in figure 7.12-(4). Thus, the temperature kept on decreasing, and the pressure in the
combustion chamber reached its peak value, and started to be lower than the pressure in the injector, so that the fuel velocity direction changed back to outward flowing from the injector to the combustion chamber as shown in figure 7.12-(3). From then on, the methane in the injector started slowly leaking outward from the nozzle to the combustion chamber. As the pressure in the combustion chamber decreased, the pressure in the injector also decreasing correspondingly, but remained a little higher than the pressure in the combustion chamber, so the leakage continued. Because the temperature has decreased to a very low value, the chemical reaction speed at this low temperature becomes very low. Thus, the methane that leaks from the injector at this low chemical reaction speed in the late phase of the cycle cannot be burned. Figures 7.12-(5) and 7.12-(6) shows the leakage growth at 3.2 ms and 6.3 ms.

At time $t=2.1$ ms in figure 7.12-(2), it can be seen that the jet was broken into two separate parts of front and tail by fast combustion in the middle part of the jet. This is because at the front of the jet, the mixture is too lean, and at the tail of the jet, the temperature is low, so the combustion speeds at both of these two parts are lower than those in the middle part of the jet. Thus, the jet was separated by combustion into the front and tail parts. At time $t=2.4$ ms in figure 7.12-(3), it can be seen that these two parts became smaller, indicating that they were separately involved in combustion because they were still located in relatively high temperature regions. At time $t=2.7$ ms in figure 7.12-(4), the front of the jet disappeared and only a little bit of the tail of the jet remained. To discover if the final part of the fuel was combusted or dispersed into the neighboring cells, the lowest scale of fuel-air mixture contour was changed to a much lower value ($\phi=0.05$) to trace the leanest part of the fuel. This is shown in figure 7.14.
Figure 7.14-(1) shows that at time $t=2.7$ ms, there was no indication of dispersion for the methane at the front of the jet under the exaggerated legend scale for showing the very lean fuel air mixture, which means it should be consumed by combustion. However, at time $t=3.2$ ms in figure 7.14-(2), a part of the tail for the fuel jet was still remaining near to the injector wall because of the dispersion under the exaggerated legend, although it can not be shown at the normal legend in figure 7.12-(5). This is because at this late combustion time, the temperature had already decreased to a low level, and the local mixture became too lean because of dispersion. Also the cold injector wall prohibited combustion nearby. So this small amount of the fuel would remain as unburned hydrocarbon emissions.

In a real engine application, because of the downward movement of the piston, the pressure drop in the cylinder after it reaches the peak value can be higher than this simulation,
which leading to the trend of more leakage from the injector through the nozzle. The amount of
the leakage can be estimated as:

\[ \Delta m = \frac{V_{sac}}{R T_n} (P_{max} - P_{BDC}) \]

where: \( V_{sac} \) is the sac volume of the injector

\( T_n \) is the injector gas temperature

\( R \) is the gas constant of the fuel.

\( P_{max} \) and \( P_{BDC} \) is the peak pressure in cylinder and pressure at BDC.

So it can be seen that the leakage of the gas fuel from the injector should be proportional
to the size of the sac volume. The smaller the sac volume is, the less leakage there will be. But
for the engine application, since the pressure drop is earlier than the temperature drop because of
the piston movement, some of this leaked fuel might be burned or partially burned by the high
temperature inside the cylinder.

7.6 Summary

This chapter has presented simulation results for methane injection by a bare glow plug
and by a shielded glow plug. In both cases, comparison with experimental results confirms that
the glow plug discretized model and the gas sub-layer model together produce results that are in
excellent agreement with experimental results. Simulations were also carried out to explore the
benefits of multi-pulse injection on ignition and to study the effect of leakage from the injector
nozzle after injector pintle shut-off. The following chapters will present the conclusions of the
overall study as well as recommendations for future work.
Chapter 8

Conclusions

This chapter summarizes the conclusions for this study under several headings, including combustion chamber swirl generation and characteristics, natural gas injection, glow plug models and natural gas ignition and combustion.

8.1. Characterization of the Combustion Chamber Apparatus

The first part of the simulation work characterized the combustion chamber apparatus used for experimental studies.

Numerical simulation confirms the experimental results that the difference between the in-cylinder pressure and the combustion chamber pressure was negligible and that the time delay associated with the flow through the connecting passage was also negligible.
The calculated swirl angular velocities were 484 rad/sec (4621 rpm) at TDC and 380.3 rad/sec (4621 rpm) at 10°CA ATDC, which showed satisfactory agreement with the experimental results.

The angular velocity profile calculated for the constant volume combustion chamber is different from the one calculated by the Bessel function based model embedded in the KIVA-3V code. The swirl profile in KIVA was modified to facilitate future simulation of experimental results obtained using the constant volume combustion chamber.

8.2. Simulation of Internal Flow in the Natural Gas Fuel Injector

The second phase of simulation studied the internal flow in the natural gas fuel injector using the poppet valve model. The injector exit plane flow provides the input boundary conditions for the glow plug ignition and combustion model.

8.2.1. Poppet Valve Model

The poppet valve model computes spatially and temporally the velocity and pressure profiles at the injector nozzle exit. The simulation result has good agreement with experimental data in the mass flow rate and the jet penetration length.

The core temperature of the injected methane jet is reduced to below 360 K from the original 400 K of temperature due to isentropic expansion. In the simulation, the methane fuel is injected into an 850 K environment. There is only a very thin outside layer in which air is entrained to make a flammable zone, so the mixing of injected methane with air is not easily accomplished. Without good mixing, methane is even more difficult to auto ignite. Note that
chemical kinetic limitations also make auto ignition difficult. As a result of these two factors, some form of ignition assistance is required.

It takes about 0.8 ms after the start of injection for the flow in the injector to be stabilized. The pressure and velocity stabilization is faster than the temperature stabilization. The flow is choked at the centerline of the nozzle exit with a single hump velocity profile. However, the exit velocity at the centerline of the nozzle varies 11% from the beginning of the injection to 0.8 ms after the injection when the flow is stabilized.

Compared to the velocity and pressure boundary conditions, although the poppet valve model has the similar steady state of the flow characteristics after the injection reaches steady after 0.8 ms, it has significant differences in flow parameters during the transient state for the early stage of the injection. These flow parameters are the important factors affecting the ignition delay time, such as the time for the jet to reach the glow plug, velocity when jet reaching the glow plug, the historical change of fuel-air equivalence ratio near glow plug surface, the transient mass flow rate, and they. Thus, these transient state differences result the different ignition delay for the poppet valve model compared to the velocity and pressure boundary conditions.

8.2.2. Simulation of Natural Gas Injection

The flow is choked at the exit of the nozzle when the nozzle diameter is larger than the critical value (about 0.34 mm), but it becomes subsonic when the nozzle diameter is smaller than the critical value because of wall friction effects.
A small nozzle size has a lower mass flow rate, which in turn results in less jet penetration. But it has a larger flammable region and a higher temperature, both of which benefit ignition.

Strong swirl improves the fuel-air mixing, especially in the region downstream of the glow plug.

A jet attachment phenomenon at the back of the glow plug helps to increase the size of the flammable region and lengthen the mixture’s residence time adjacent to the glow plug. Both benefit autoignition. Under the swirl conditions simulated, glow plug placement 15° upstream to the swirl from the jet exit is the best position for autoignition in terms of shorter ignition delay and better combustion stability.

The round shield surrounding the glow plug decreased the flow velocity passing the glow plug to about 1/3 compared to the bare glow plug, thus increasing the residence time, which benefits the natural gas autoignition.

8.3. Simulation of Glow Plug Assisted Ignition

8.3.1. Glow Plug Ignition Model

The model representing the glow plug has to be discretized for consideration of glow plug surface transient temperature change at different locations.

A quasi-3d solid glow plug discretized model can describe the transient heat transfer, and adequately represents the thin layers of the heat penetration. The local temperature difference
due to the cold gas jet impinging onto the surface of the glow plug can be considered with this described model.

Only a very thin layer of gas surrounding the glow plug ($10^{-6}$ m) can be efficiently heated to high temperature, and therefore ignition occurs in this thin layer.

The virtual sub-layer model sub-divides the gas cells surrounding the glow plug into very thin sub-layers, Within each sub-layer, complicated physical processes are considered, such as chemical reaction, heat conduction, and mass diffusion. The virtual sub-layer model can simulate ignition without significantly increasing computational time and load.

A quasi-3d solid glow plug discretized model working together with the virtual sub-layer model successfully simulates the glow plug ignition process. It can predict the ignition delay time and locate the ignition starting points.

8.3.2. Simulation of Glow Plug Ignition Processes

Simulation of bare glow plug ignition shows good agreement with the experimental results. It can correctly predict the ignition delay time and locate the ignition starting points.

Simulation of methane ignition over a shielded glow plug confirms the conclusion from the flow simulation that the decrease of the velocity passing the glow plug and the increase of the residence time of the flammable mixture to the glow plug benefits the ignition. The ignition location is as expected at the flammable region with the longest residence time adjacent to the glow plug. Flame first propagates inside the shield around the glow plug, and then propagates outside of the shield through the slot and ignites the main jet.
Simulation of multi-pulse injection shows successful ignition and flame propagation from the first injected jet to the second one. The proper interval time between multiple pulses is an important parameter for successful ignition of the following injections.

Simulation of leakage from the injector nozzle after pintle shut off shows that the jet separated into front and tail parts because of the fast ignition at the middle of the jet. All the fuel at the jet front is finally burned, but a small amount of the fuel at the tail which is close to the cold injector wall cannot be burned and remains as unburned hydrocarbon emissions. After the pintle shuts off, with the temperature and pressure becoming smaller at the end of combustion in the combustion chamber, the fuel is leaking out from the injector into the combustion chamber through the nozzle, where it cannot be burned due to the low temperature. It also remains as unburned hydrocarbon emission.

8.4. Summary

In summary, the contribution of glow plug discretized model and the virtual gas sub-layer model are the first reported models to reveal the physics of the glow plug ignition process and successfully simulate glow plug ignition of natural gas. As well, the poppet valve model is the first reported model to successfully simulate the internal flow in the natural gas fuel injector. The results obtained with these models show how future direct injection natural gas engines can be optimized.
Chapter 9

Recommendations

With the lessons learned in this study many suggestions and recommendations, especially for simulation work, are made for future research on the topic of the natural gas direct injection engine. This chapter introduces these recommendations for future work.

9.1. Incorporation of a Two Step Kinetic Reaction Model

KIVA-3V has a built-in one-step kinetic reaction model that has been tuned for use with a variety of conventional liquid fuels. It works well in researching and evaluating the overall parameters of engine performance associated with combustion, such as pressure, temperature change, combustion efficiency, output power, etc. The advantage is affordable computation by a much simplified combustion process coupled with computational fluid dynamics. Since it is only one-step reaction covering a large range of temperatures (850-2500K), it is difficult to tune over the entire temperature range and therefore can generate errors for the low or the high temperature
end of the range. This can be seen in the kinetic reaction tuning for methane described in Appendix G.

For the ignition study, the interest is focused more on the temperature range of 850-2000K rather than the temperature range of 2000-2500K for the study of main combustion. A two-step kinetic reaction model divides the single step of methane combustion (CH₄ directly into CO₂) into two steps. These two steps include a first reaction step for methane to be oxidized into the intermediate product carbon monoxide (CO), which occurs at a relatively low temperature, and a second step of further oxidation of CO into CO₂ at a relatively high temperature. This two-step model provides more accurate chemical reaction details at both low and high temperatures, which will facilitate the tuning of the kinetic model and reduce the simulation error for ignition and combustion over wider range of temperatures. Mtui and Hill [1998] introduced their implementation of a two-step methane oxidation scheme recommended by Westbrook and Dryer [1981] in their simulation work and had satisfactory agreement with their experimental results.

9.2. Injection Nozzle Redesign: Combination of Small and Larger Nozzles

As discussed in section 4.3.1, a very small nozzle of 0.15 mm diameter forms a jet with more air entrained, because it does not overlap any adjacent jet. More air entrainment creates a larger flammable region and a high mixing temperature. Ignition benefits as a result. However, due to the large friction from the wall of the small nozzle on the flow, the jet is restricted to subsonic flow with an exit Mach number of 0.4. The small mass flow rate (1/20 of the mass flow rate for an 0.5 mm diameter nozzle) cannot provide enough fuel within the effective injection period. A new injection nozzle concept is proposed to combine the favorable ignition
characteristics of a small nozzle with the fuel flow capability of the larger nozzles such that both requirements of fast ignition and injection of adequate fuel in a short time can be met.

In order to implement the small nozzle/large nozzle concept, the glow plug location needs to be investigated in order to ignite the jet from small nozzle at proper time. The injection angle between the small ignition nozzle and its neighboring large nozzles will be another very important parameter, since it determines cooling effects to the jet issued from the small nozzle as well as to the glow plug. Many other parameters also need to be researched such as the lowest temperature required for the bare glow plug, the necessity of the shield, the injection period, and the nozzle hole orientation.

9.3. Research on Glow Plug Shield Design

A full or partial shield around a glow plug can increase the residence time of the fuel air mixture adjacent to the glow plug, and maintain the glow plug at higher temperature by preventing direct exposure of the glow plug to the surrounding cold swirling air. It can also increase the combustion stability at different engine working conditions. These benefits all arise because the shield significantly changes the flow pattern around the glow plug. Shield dimension, shape, and orientation have a strong impact on the flow pattern, and thus need to be studied intensively to explore all possibilities and optimize the most promising configurations.

This thesis studied the shape of a small round shield. Other possible shapes and dimensions for the shield can also be explored in the future, such as a larger round shield surrounding the glow plug, an L shaped shield before the glow plug, both of which were utilized in previous experimental studies at ERDL.
For the round shield, the size of the hole and its orientation need to be studied. For this research, the shield openings (slot) was turned 40.7° towards the jet and this configuration was studied by simulation. Different turning angles will result in different amounts of fuel being directly injected into the shield, thus changing the time for the fuel air mixture to reach the glow plug, and also changing the flow velocities surrounding the glow plug. These changes will have a great impact on autoignition. A test matrix of turning angles and the size of the slots can be studied for optimization. Use of multiple slots can also be researched, to see whether or not flame propagation from the inside of the shield out to the combustion chamber will benefit from a suitable internal flow generated inside the shield.

9.4. Implementation of Multi-pulse Injection for Improved Ignition and Combustion

As introduced in section 7.4, multi-pulse injection can shorten the ignition delay time, reduce the rate of pressure rise, and may possibly reduce the amount of the gaseous fuel directly impinging onto the cold walls of the combustion chamber. Several important parameters need to be further researched, such as the length of the first injection pulse, the shut-off interval time between the two injection pulses, the number of the total injection pulses and their lengths, etc. This multi-pulse injection technique may be constrained by the injector hardware capability, e.g., the ability to respond at high speed.

The injection length of the first pulse will determine the ignition delay time. A first injection pulse that is too short may not provide adequate residence time of the fuel adjacent to the glow plug, since the swirl will blow the jet downstream away from the glow plug.
The shut-off interval time between the two pulses needs to be optimized. Too short interval may quench the flame before combustion of the previous jet is sufficiently established. On the other hand, too long an interval may not ignite the following jet after the main combustion of the previous jet finishes.

The number of the total injection pulses and their lengths can be determined by the required amount of the fuel to be injected, as well as by the jet penetration length under combustion, so that a minimum of fuel will be impinging onto the combustion chamber.

### 9.5. Research on Improved Mixing through Use of Elliptical Nozzles

Some preliminary research has been done for methane gas injection through an elliptical nozzle. This is described in Appendix H, which shows the axis-switching phenomenon. However, the simulation result does not provide the evidence of improved mixing effect compared to the equivalent round nozzle. More cases of different nozzle sizes and aspect ratios of elliptical nozzles under different injection pressures should be studied to further understand the flow characteristics of the elliptical nozzles.

### 9.6. Research on Pintle Valve Model

The poppet valve model does not have the same shape and moving direction as the real injector pintle shown in figure 2.2, therefore, a new pintle valve model was developed to study the differences of the natural gas flow between the two models. Many modifications were made by the author in both the mesh generator and the KIVA main code for the pintle valve model. They are listed in appendix A.
Some preliminary research has been done to compare the methane flow parameters between the pintle valve model and the poppet valve model; it shows that the pintle valve model has the similar transient flow characteristics but with less restriction to the flow compared to the poppet valve model. The details are introduced in appendix I. More cases of methane injection and ignition should be conducted with the pintle valve model for comparison to the poppet valve model and for the further development of the pintle valve model.

9.7. Summary

As a summary, with the code and model well developed for the injector model and glow plug ignition model after this Ph.D. research, more complicated cases and possible combinations can be conducted with some necessary modifications of the mesh generation for the study of the natural gas injection and ignition, which are the two technical challenges for the direct injection natural gas (DING) engines.
References


2. Aesoy, V., and Valland, H., Hot surface thermal ignition of a transient gas-jet in a constant volume combustion bomb, University of Trondheim, Norway, 1996


40. Sun, M., Simulation of natural gas injection into a constant-volume chamber, internal report, Engine Research and Development Laboratory, University of Toronto, 1999.


45. www.NGK.de

Appendix A

List of Modifications to KIVA

To generate complicated geometry, e.g. a glow plug shield with a slot turned at a certain angle, many modifications have been applied on the mesh generator for the original KIVA code. To model the internal flow within the fuel injector as well as the glow plug ignition and combustion process, many modifications have been made on the KIVA main solver as well. This appendix briefly lists these modifications for further research on the KIVA code for natural gas fueled engines.
## A.1. List of Modifications on the Mesh Generator

Table A.1 List of modifications on the mesh generator

<table>
<thead>
<tr>
<th>No.</th>
<th>Modification</th>
<th>Subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>set multzsqsh=1 for the computation of 'Simple Structure of Glow Plug Shield'</td>
<td>k3pre</td>
</tr>
<tr>
<td>2</td>
<td>Change to make flags of the vertices / faces for the patching of ghost working fine for 'KIVA3.f'</td>
<td>Connfd, connlr</td>
</tr>
<tr>
<td>3</td>
<td>Adding following block due to patch the curvature faces.</td>
<td>connfd, connlr</td>
</tr>
<tr>
<td>4</td>
<td>Change to consider if the patching block has already rotated an angle 'alpha' along z-axis, need to rotate back to consider the new Y projection values. After finding the cell and coordinates, need to rotate to the original state.</td>
<td>connfd, connlr</td>
</tr>
<tr>
<td>5</td>
<td>Change due to patch the curvature faces. Add case of 'icoor=-1' for patching curvature faces.</td>
<td>patch</td>
</tr>
<tr>
<td>6</td>
<td>Change due to patch the curvature faces. Adding two more cases for if patching for curvature faces</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1. ixyz=-1, patching blk is block1, and use left face to patch curvature faces of block2 right face.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. ixyz=-2, patching blk is block1, and use right face to patch curvature faces of block2 left face.</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Add following in order to not re-shape some of the blocks for the combustion chamber case.</td>
<td>reshapeb</td>
</tr>
<tr>
<td>8</td>
<td>Change to disable the conditional statements.</td>
<td>reshapeb</td>
</tr>
<tr>
<td></td>
<td>For adding glow plug (ghost block) reshaped to the specific original block, which is cylindrical block, disable following conditional statement which does not allow to reshape the cylindrical blocks.</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Add this part to generate a cylindrical block with a Cartesian coordinate symmetric along x-axis instead of z-axis originally generated by K3PREP</td>
<td>setup</td>
</tr>
<tr>
<td></td>
<td>Change to NTYPE=6 for this case.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------</td>
<td>---</td>
</tr>
<tr>
<td>10</td>
<td>This change was applied to the generation of a nozzle for injection simulation, the generation of combustion chamber for simulation of the swirl formation.</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Insert this part for making the elliptical section instead of original round one.</td>
<td>setup</td>
</tr>
<tr>
<td>12</td>
<td>Add this part to generate a cylindrical block with a Cartesian coordinate symmetric along y-axis instead of x or z-axis originally generated by K3PREP. Change to NTYPE=7 for this case.</td>
<td>setup</td>
</tr>
<tr>
<td>13</td>
<td>Add NTYPE=2.5 case for shield GP Add NTYPE=8.0 case for no-central-axis cylinder with uneven peripheral segment length, for the case of rotated shield</td>
<td>setup</td>
</tr>
<tr>
<td>14</td>
<td>Change angle of 135 to 165, 225 to 195 correspondingly for a new glow plug mesh structure by adding two cases if NTYPE=8.0.</td>
<td>setup</td>
</tr>
<tr>
<td>15</td>
<td>Add a new subroutine “cylindric” to generate uneven cylindrical mesh</td>
<td>cylindric (NEW)</td>
</tr>
<tr>
<td>16</td>
<td>Add a new subroutine “curvline” to change the cylindrical block outline (r-z plane) from a straight line (cylinder shape) to any shape of a curved line</td>
<td>curvline (NEW)</td>
</tr>
<tr>
<td>17</td>
<td>Add a new subroutine “rotate” to rotate blocks along the central line of z-axis</td>
<td>rotate (NEW)</td>
</tr>
<tr>
<td>18</td>
<td>Add a new subroutine “propfce” for pintle model to shape the each pintle surface (face) to a user-specified silhouette, and is applicable when the surface is not perfectly flat.</td>
<td>propfce (NEW)</td>
</tr>
</tbody>
</table>
### A.2. Modifications on the Main Solver

Table A.2 List of modifications on the main solver

<table>
<thead>
<tr>
<th>No.</th>
<th>Modification</th>
<th>Subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Add total energy conservation</td>
<td>bcccin</td>
</tr>
<tr>
<td>2</td>
<td>Change pap to pceffne(i4), and i4l(f)(b)ppres to i4lpres for total energy</td>
<td>bcpgrad, bcpexd, bcresp,</td>
</tr>
<tr>
<td></td>
<td>conservation</td>
<td>setupbcd</td>
</tr>
<tr>
<td>3</td>
<td>Modify Mach number by average inlet velocity</td>
<td>bcccin</td>
</tr>
<tr>
<td>4</td>
<td>Define all variables as real</td>
<td>bcccin</td>
</tr>
<tr>
<td>5</td>
<td>Set no friction at pressure inflow boundary at wall position</td>
<td>lawall</td>
</tr>
<tr>
<td>6</td>
<td>Modify to incorporate with glow plug model for the thin boundary layers.</td>
<td>lawall</td>
</tr>
<tr>
<td>7</td>
<td>Add new output for 1) fuel/air equivalence ratio 2) Mach number</td>
<td>tecconv</td>
</tr>
<tr>
<td>8</td>
<td>Solving the memory usage keep on increasing problem.</td>
<td>tecconv</td>
</tr>
<tr>
<td></td>
<td>The original code made the memory usage increasing for each writing to output file.</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Modify to introduce a new file management system, separate input/output files into different 3 folders</td>
<td>pltgmv, rinput</td>
</tr>
<tr>
<td>10</td>
<td>Add swirl when rpm=0 for combustion bomb situation.</td>
<td>setup</td>
</tr>
<tr>
<td>11</td>
<td>Add to calculate the mass for each species in each different zones by geometric definition. Result is written into a new file 'otape9'.</td>
<td>globbal</td>
</tr>
<tr>
<td>12</td>
<td>Add the analytical temporary results written to a new file of otape10</td>
<td>globbal</td>
</tr>
<tr>
<td>13</td>
<td>The original code cannot read in all the digits input, increase the reading digits from f10.5 to f12.5</td>
<td>rinput</td>
</tr>
<tr>
<td>14</td>
<td>Change nctap8, nclast, nemon to 6 digits from original 5 digits, so the code will not dump early and can run longer time.</td>
<td>newcyc itape5</td>
</tr>
<tr>
<td>15</td>
<td>Change the system default of real number precision from 4 bytes to 8 bytes.</td>
<td>comkiva bdchmqgm neweyc</td>
</tr>
<tr>
<td></td>
<td>Description</td>
<td>Subroutine/Parameter</td>
</tr>
<tr>
<td>---</td>
<td>-----------------------------------------------------------------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>16</td>
<td>Modification for poppet valve model in the fuel injector. Change to allow valve motion with no crankshaft motion. This case is distinguished by a new input parameter crankmov=0.0</td>
<td>adjvalve rinput</td>
</tr>
<tr>
<td>17</td>
<td>Add a new subroutine “adjpintle” for pintle model. pintle=1/0 to call/bypass the model</td>
<td>adjpintle</td>
</tr>
<tr>
<td>18</td>
<td>Modifications for incorporating with pintle model.</td>
<td>kiva, rinput, adjvalve</td>
</tr>
<tr>
<td>19</td>
<td>Add criterion of Tcell&lt;2000 to bypass turbulent mixing-control chemistry</td>
<td>chem</td>
</tr>
<tr>
<td>20</td>
<td>Set zp(npn)=0 for making GP case work</td>
<td>chem</td>
</tr>
<tr>
<td>21</td>
<td>Add a new subroutine “locategp” to locate the glow plug position in order to flag the boundary cells for the glow plug</td>
<td>locategp</td>
</tr>
<tr>
<td>22</td>
<td>Add a new subroutine “setupgp” to setup the glow plug model by assigning all the GP values.</td>
<td>setupgp</td>
</tr>
<tr>
<td>23</td>
<td>Add a new subroutine “gpinitiate” to initiate glow plug additional properties, because some of the properties cannot be set at 'setupgp'</td>
<td>gpinitiate</td>
</tr>
<tr>
<td>24</td>
<td>Add a new subroutine “glowplug” to overall handle the glow plug ignition and combustion by calling other new added subroutines glowplg=1/0 to call/bypass this model</td>
<td>glowplug</td>
</tr>
<tr>
<td>25</td>
<td>Modify to set up glow plug temperature, besides using law of wall for other boundaries. fixtemp=0.0 to by pass this option.</td>
<td>exdif</td>
</tr>
<tr>
<td>26</td>
<td>Add a new subroutine “chemgp” to model the chemical reaction within the virtual gas sub-layers</td>
<td>chemgp</td>
</tr>
<tr>
<td>27</td>
<td>Add a new subroutine “gpheattr” to model the heat transfer process within discretized GP cells and virtual gas sub-layers, including conduction loss to base and radiation loss to environment</td>
<td>gpheattr</td>
</tr>
<tr>
<td>28</td>
<td>Add a new subroutine “gpmassdf” to model the mass diffusion process within virtual gas sub-layers by applying Fick's law</td>
<td>gpmassdf</td>
</tr>
<tr>
<td>29</td>
<td>Add pure conduction at glow plug wall position, i.e. conduction between first sub-layer of gas with the left gas cell. wallcond=0.0 to turn off the option</td>
<td>gpd, gpheattr</td>
</tr>
<tr>
<td></td>
<td>Description</td>
<td>Subroutine/Function</td>
</tr>
<tr>
<td>---</td>
<td>-----------------------------------------------------------------------------</td>
<td>---------------------</td>
</tr>
<tr>
<td>30</td>
<td>Add a new subroutine “gpkeypty” to calculate the 3 KEY properties for the virtual gas sub-layers: specific energy, density, and fraction of each species.</td>
<td>gpkeypty (NEW)</td>
</tr>
<tr>
<td>31</td>
<td>Add a new subroutine “gpupdate” to update all the other properties for the virtual gas sub-layers based by the 3 key properties.</td>
<td>gpupdate (NEW)</td>
</tr>
<tr>
<td>32</td>
<td>Add a new subroutine “gpleftcell” to evaluate the new properties after left gas cell interact with neighbor cells.</td>
<td>gpleftcell (NEW)</td>
</tr>
<tr>
<td>33</td>
<td>Add a new subroutine “gppbalance” to balance the pressure between each sub-layers for the mass redistribution process.</td>
<td>gppbalance (NEW)</td>
</tr>
<tr>
<td>34</td>
<td>Add a new subroutine “gpdt” to optimize the time step for glow plug chemical reaction, heat transfer, and mass diffusion.</td>
<td>gpdt (NEW)</td>
</tr>
<tr>
<td>35</td>
<td>Add a new function “hhisp” to calculate the specific energy and specific enthalpy for each species at a given temperature.</td>
<td>hhisp (New)</td>
</tr>
<tr>
<td>36</td>
<td>Add a new subroutine “linrsolvm” to solve the linear equation of band diagonal systems for mass diffusion model with backward implicit method.</td>
<td>linrsolvm (NEW)</td>
</tr>
<tr>
<td>37</td>
<td>Add a new subroutine “linrsolvh1” to solve the linear equation of band diagonal systems for heat transfer model between virtual gas sub-layers with backward implicit method.</td>
<td>linrsolvh1 (NEW)</td>
</tr>
<tr>
<td>38</td>
<td>Add a new subroutine “linrsolvh2” to solve the linear equation of band diagonal systems for heat conduction model between discretised glow plug cells with backward implicit method.</td>
<td>linrsolvh2 (NEW)</td>
</tr>
<tr>
<td>39</td>
<td>Add a new subroutine “bandec” to mathematically solve the linear equation of band diagonal systems.</td>
<td>bandec (NEW)</td>
</tr>
<tr>
<td>40</td>
<td>Add a new subroutine “threepi” to conduct 3-points interpolation for finding the temperature based on the specific energy, improved from original 2-points interpolation.</td>
<td>threepi (NEW)</td>
</tr>
</tbody>
</table>
Appendix B

Bessel Function

The swirl intensity is calculated by a Bessel function embedded in the KIVA code. However, because of the different mechanisms of swirl generation between the combustion chamber in this research and in conventional engine applications, the swirl velocity profiles for the combustion chambers in this research must also be different. Thus, the KIVA suggested swirl velocity profile has to be modified in order to accommodate the new combustion chamber situation in this research. This appendix introduces the embedded Bessel function in the KIVA code and the modified inputs for the new swirl velocity profile for the combustion chamber.
**B.1. Introduction to Bessel Function**

The general formula for the Bessel function of the first kind of order two is given by:

\[ j_2(x) = \frac{2}{x} \cdot j_1(x) - j_0(x) \]

where: \( j_0(x) \) is the Bessel function of the first kind of order 0.

\[ j_0(x) = \frac{r_1 + x^2 (r_2 + x^2 (r_3 + x^2 (r_4 + x^2 (r_5 + x^2 r_6))))}{s_1 + x^2 (s_2 + x^2 (s_3 + x^2 (s_4 + x^2 (s_5 + x^2 s_6))))} \quad \text{when } -8 < x < 8 ; \]

\[ j_0(x) = \sqrt{\frac{c_1}{|x|}} \cdot \left\{ \left[ \cos(|x| - c_2) \cdot (p_1 + \frac{64}{x^2} (p_2 + \frac{64}{x^2} (p_3 + \frac{64}{x^2} (p_4 + \frac{64}{x^2} p_5)))) \right] - \left[ \frac{8}{|x|} \cdot \sin(|x| - c_2) \cdot (q_1 + \frac{64}{x^2} (q_2 + \frac{64}{x^2} (q_3 + \frac{64}{x^2} (q_4 + \frac{64}{x^2} q_5)))) \right] \right\} \]

when \( x \leq -8 \) or \( x \geq 8 \).

\( j_1(x) \) is the Bessel function of the first kind of order 1.

\[ j_1(x) = \frac{r_1 + x^2 (r_2 + x^2 (r_3 + x^2 (r_4 + x^2 (r_5 + x^2 r_6))))}{s_1 + x^2 (s_2 + x^2 (s_3 + x^2 (s_4 + x^2 (s_5 + x^2 s_6))))} \cdot x \quad \text{when } -8 < x < 8 ; \]

\[ j_1(x) = \frac{x}{|x|} \cdot \sqrt{\frac{c_1}{|x|}} \cdot \left\{ \left[ \cos(|x| - c_2) \cdot (p_1 + \frac{64}{x^2} (p_2 + \frac{64}{x^2} (p_3 + \frac{64}{x^2} (p_4 + \frac{64}{x^2} p_5)))) \right] - \left[ \frac{8}{|x|} \cdot \sin(|x| - c_2) \cdot (q_1 + \frac{64}{x^2} (q_2 + \frac{64}{x^2} (q_3 + \frac{64}{x^2} (q_4 + \frac{64}{x^2} q_5)))) \right] \right\} \]

when \( x \leq -8 \) or \( x \geq 8 \).

The values of the above constants in the Bessel functions are listed in table B.1 and B.2.
Table B.1 The values of the constants in $j_0(x)$

<table>
<thead>
<tr>
<th>Subscript</th>
<th>$p$</th>
<th>$q$</th>
<th>$r$</th>
<th>$s$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>-1.562499995e-02</td>
<td>5.7568490574e+10</td>
<td>5.7568490411e+10</td>
<td>0.636619772</td>
</tr>
<tr>
<td>2</td>
<td>-1.098628627e-03</td>
<td>1.430488765e-04</td>
<td>-1.3362590354e+10</td>
<td>1.0295329850e+09</td>
<td>0.785398164</td>
</tr>
<tr>
<td>3</td>
<td>2.734510407e-05</td>
<td>-6.911147651e-06</td>
<td>6.5161964070e+08</td>
<td>9.4946807180e+06</td>
<td>N/A</td>
</tr>
<tr>
<td>4</td>
<td>-2.073370639e-06</td>
<td>7.621095161e-07</td>
<td>-1.1214424180e+07</td>
<td>5.9272648530e+04</td>
<td>N/A</td>
</tr>
<tr>
<td>5</td>
<td>2.093887211e-07</td>
<td>-9.349451520e-08</td>
<td>7.7392330170e+04</td>
<td>2.6785327120e+02</td>
<td>N/A</td>
</tr>
<tr>
<td>6</td>
<td>N/A</td>
<td>N/A</td>
<td>-1.8490524560e+02</td>
<td>1.0</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Table B.2 The values of the constants in $j_1(x)$

<table>
<thead>
<tr>
<th>Subscript</th>
<th>$p$</th>
<th>$q$</th>
<th>$r$</th>
<th>$s$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>4.687499995e-02</td>
<td>7.2362614232e+10</td>
<td>1.44725228442e+11</td>
<td>0.636619772</td>
</tr>
<tr>
<td>2</td>
<td>1.831050000e-03</td>
<td>-2.002690873e-04</td>
<td>-7.8950592350e+09</td>
<td>2.30053517800e+09</td>
<td>2.356194491</td>
</tr>
<tr>
<td>3</td>
<td>-3.516396496e-05</td>
<td>8.449199096e-06</td>
<td>2.4239685310e+08</td>
<td>1.85833047400e+07</td>
<td>N/A</td>
</tr>
<tr>
<td>4</td>
<td>2.457520174e-06</td>
<td>-8.822898700e-07</td>
<td>-2.9726114390e+06</td>
<td>9.94474339400e+04</td>
<td>N/A</td>
</tr>
<tr>
<td>5</td>
<td>-2.403370190e-07</td>
<td>1.057874120e-07</td>
<td>1.5704482600e+04</td>
<td>3.76999139700e+02</td>
<td>N/A</td>
</tr>
<tr>
<td>6</td>
<td>N/A</td>
<td>N/A</td>
<td>-3.0160366060e+01</td>
<td>1.0</td>
<td>N/A</td>
</tr>
</tbody>
</table>

B.2. Angular velocity chosen

The swirl velocity $V(\rho)$ at radius $r$ is calculated by the following Bessel functions embedded in KIVA code:

$$V(r) = A \cdot \frac{P_s \cdot j_1\left(\frac{r}{R} \cdot P_s\right)}{j_2(P_s)}$$

where: $A$ and $P_s$ are two inputs for the swirl profile,

$A$ determines the amplitude of the swirl velocity;
$P_s$ determines the shape of the swirl velocity profile, $0 < P_s < 3.84$.

The trend of $P_s$ determining the shape of swirl velocity profile is shown in figure B.1.

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

Figure B.1  The trend of $P_s$ determining the shape of swirl velocity profile. Amplitude $A$ is chosen as a constant of 18.11.

The original KIVA code suggests $A=18.11$ and $P_s=3.11$ for the conventional engine application. The new values of $A=27.23$ and $P_s=2.0$ were chosen for calculating the swirl velocity profile for the combustion chamber in the ERDL combustion bomb. This change results in the new swirl velocity profile shown in figure 3.9, where it is compared to the KIVA suggested profile and swirl simulation results for combustion chamber in the ERDL combustion bomb.
Appendix C

Total Energy Conservation at Pressure Boundary Condition

The pressure boundary condition in the original KIVA code overestimates the extent of expansion, giving a very low temperature. The calculated temperature could go below 190K at the central cold core of the methane jet expanding from the high pressure fuel reservoir to the low pressure combustion chamber environment, as shown in figure C.1 by the research from Sun [1999], and figure C.2 from my previous research work [Cheng and Wallace, 2004].

If the gas pressure at the high pressure reservoir side is increased further, the core expansion temperature decreases linearly to a temperature below 100K, which is not a physically realistic result since this temperature crosses the methane phase change zone from gas to liquid, suggesting that liquid fuel should appear in the expansion jet. However, this phenomenon has not been observed in previous research.
Figure C.1 Expansion temperature computed by the original KIVA code with a pressure boundary condition [Sun, 1999]. The jet core temperature is 186K at the nozzle outlet.

Figure C.2 Temperature profile computed using the original KIVA code with a pressure boundary condition [Cheng, S.X. and Wallace, 2004]: Temperature profile (11MPa, 400K methane expanded to 4MPa, 850K in the combustion chamber). The core temperature of the methane jet is below 190 K at the nozzle outlet.
Doubting this result led to further research into the original KIVA code, applying the pressure boundary condition to a simple round duct case that can be easily treated by fundamental thermodynamic principles. The schematic of pressure boundary condition and the physics of the flow process from reservoir to duct inlet are illustrated in figure C.3.

Figure C.3  Schematic of the pressure boundary condition and the physics of the flow process from reservoir to duct inlet

Figure C.4 shows the results from the original KIVA code, which treats the pressure input for pressure boundary condition as the static pressure $P$ at the duct inlet, even though it is actually the reservoir stagnation pressure $P_0$. Thus, for an input pressure of 11 MPa, the velocity is accelerated to a very high value (900 m/s) at the duct inlet, which is physically unrealistic. Also, to keep the total energy conserved, the computed temperature dropped down to 150K.
The actual static pressure $P$ at the duct inlet for a giving stagnation pressure $P_0$ can be derived from gas dynamics [Liepmann and Roshko, 1957]. In an adiabatic flow, the energy equation for a perfect gas is:

$$\frac{1}{2}u^2 + c_p T = c_p T_0$$  \hspace{1cm} \text{Equation (C-1)}$$

From this total energy equation, the following equations can be derived:

$$\frac{T_0}{T} = 1 + \frac{\gamma - 1}{2} M^2$$  \hspace{1cm} \text{Equation (C-2)}$$

$$\frac{p_0}{p} = \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\gamma/(\gamma - 1)}$$  \hspace{1cm} \text{Equation (C-3)}$$

$$\frac{p_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\gamma/(\gamma - 1)}$$  \hspace{1cm} \text{Equation (C-4)}$$
KIVA was modified so that the input values of $T_0$ and $P_0$ for the pressure boundary condition are used to calculate the correct values of $T$, $P$, and $V$ at the duct inlet. The new result computed with the revised pressure boundary condition is shown in figure C.5, it gives a lower velocity at the entrance, with a lower pressure (7.2 MPa) and a reasonably higher temperature (375 K). Table C.1 details the comparison of flow parameters at inlet of the pressure boundary conditions between the original KIVA code and the modified KIVA code.

![Pressure, Temperature and Velocity along the Central Line of the Round Duct](image)

**Figure C.5** Computed gas expansion result when the modified KIVA code is applied to a simple round duct. High pressure reservoir 11 MPa, 400 K, low pressure reservoir 4 MPa, 850K.

**Table C.1** Comparison of the flow parameters at inlet plane of the pressure boundary conditions between the original KIVA code and the modified KIVA code

<table>
<thead>
<tr>
<th>Flow parameters</th>
<th>P (MPa)</th>
<th>T (K)</th>
<th>V (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>High pressure reservoir</td>
<td>11</td>
<td>400</td>
<td>0</td>
</tr>
<tr>
<td>Original KIVA code</td>
<td>11</td>
<td>150</td>
<td>900</td>
</tr>
<tr>
<td>Improved KIVA code</td>
<td>7.2</td>
<td>375</td>
<td>430</td>
</tr>
</tbody>
</table>
Applying this modified KIVA code to the combustion chamber situation, the new computed jet core temperature is increased to 350K compared to 190K from the original code.
Appendix D

Shock Wave Phenomenon

When methane is injected from the injector at a high pressure (11 MPa) to the combustion chamber at a low pressure (4 MPa), the nozzle chokes the flow at the nozzle exit and makes the flow under expansion after it reaches steady state. From equation (C-3) with the choking condition of Mach number=1, theoretical analysis shows that the pressure ratio \( P_0/P \) when choking at the nozzle exit is 1.84, which corresponds to 6.0 MPa at the nozzle exit. Therefore, at the downstream of the nozzle exit in the combustion bomb, a series of shock waves should be observed with the gas quick expansion from 6.0 MPa to 4.0 MPa. To compute these shock waves by CFD code, it requires a suitably fine mesh, which dramatically increases the computational load.
D.1. KIVA Computed Shock Waves

Figure D.1 shows the result of pressure and Mach number outside of the nozzle in the combustion bomb with a relatively finer mesh compared to the regular mesh normally used in injection and ignition simulations. The comparison of the finer mesh density to the regular mesh in the 90° sector containing the nozzle is shown in table D.1. The detailed mesh structure can be referred to figure 4.9. It can be seen that the Mach number first further increases then drops down, with the pressure jumping down quickly from 6.0 MPa to 3.5 MPa then recovered to 4.0 MPa, the chamber pressure. As KIVA is a finite difference CFD code, it cannot fully compute the discontinuity of the shock waves. Although KIVA has the tendency to smooth the shock waves, it still can analyze the shock wave phenomenon and positions if the mesh is fine enough. It may need much finer mesh than the mesh used above to further discover the shock wave behavior inside the combustion bomb.
Table D.1  Comparison of cell densities in the 90° sectors containing the nozzle for the finer mesh used in the shock wave study and the regular mesh normally used in injection and ignition simulations.

<table>
<thead>
<tr>
<th>Mesh structure</th>
<th>The regular mesh</th>
<th>The finer mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell density</td>
<td>23×24×30</td>
<td>30×48×34</td>
</tr>
</tbody>
</table>

D.2.  Comparison to FLUENT Result

FLUENT is a commercial package specialized in numerical calculation and analysis for a flow and very widely used in industry, although it is a ‘black box’ type and thus not very adaptable in the present type of research work. We compared the results from KIVA to FLUENT for simple shapes of domains and the same initial conditions. Figure D.2 shows the dimension of the domain. The comparison results in figure D.3 show that basically the results of the two codes have a satisfactory agreement to each other in terms of shock wave positions and Mach number magnitude. However, KIVA has more of a tendency to smoothen the curves of rapid changing properties because of its finite difference method compared to the finite volume method for FLUENT.
Figure D.3  Comparison results between FLUENT and KIVA. Initial condition: 11MPa to 80KPa at 297K through a 0.344mm diameter nozzle

D.3. Shock Wave Location

From the figure D.1 and figure D.3 right, it can be seen that the series of shock waves appear only over a small region in the open space which is very close to the nozzle exit plain. For the above mentioned case, it is within 2~2.5 mm downstream from the nozzle exit. The pressure is stabilized after 3 mm downstream of the nozzle exit. Normally the glow plug is placed relatively far away from this region. The glow plug is 7 mm away from the centerline of the nozzle exit when it is placed 15° upstream of the nozzle centerline as shown in figure 7.1.

Additional computations were carried out using KIVA with a simplified domain to explore the shock wave effect near the glow plug position. The dimension for this simplified domain is shown in figure D.4. Table D-2 shows the comparison of the flow parameters at 5.0 mm, 7.0 mm, and 9.0 mm downstream at the centerline of the methane jet, which was injected from 22 MPa, 400 K reservoir to 4 MPa, 850 K environment. Two mesh sizes were used in the simulations. The regular mesh has a mesh size of 0.45 mm, which is similar to the regular one.
we used in the ignition simulation in chapter 7 of this research. The fine mesh has a mesh size of 0.15 mm, which is 3 times denser than the regular mesh, which could clearly simulate the shock wave phenomenon as shown in figure D.5.

From table D-2, it can be found that the flow parameters at 5.0 mm downstream at the centerline of the methane jet only have little differences between the fine mesh and the regular mesh except the temperature. The differences of the flow parameters decrease to 0.3 % ~ 5.4 % at 7.0 mm downstream, and they further decrease to 0 % ~ 3.0 % at 9.0 mm downstream. The mesh density itself may generate these small computational differences between the fine mesh and the regular mesh. So, the shock wave may not have noticeable effects on flow parameters and thus on the ignition process in the region of more than 7 mm downstream of the methane jet from the nozzle exit.
Table D-2  Comparison of the downstream flow properties between the fine mesh and the regular mesh

<table>
<thead>
<tr>
<th>Downstream distance from nozzle exit</th>
<th>5 mm</th>
<th>7 mm</th>
<th>9 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh size</td>
<td>Regular</td>
<td>Fine</td>
<td>Regular</td>
</tr>
<tr>
<td>Mach Number</td>
<td>Value</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.74</td>
<td>0.77</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>Difference</td>
<td>--</td>
<td>-2.5 %</td>
</tr>
<tr>
<td>Pressure (Mpa)</td>
<td>Value</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3909.4</td>
<td>3902.4</td>
<td>3923.0</td>
</tr>
<tr>
<td></td>
<td>Difference</td>
<td>-0.2 %</td>
<td>--</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>Value</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>515.9</td>
<td>465.7</td>
<td>562.2</td>
</tr>
<tr>
<td></td>
<td>Difference</td>
<td>-10.8 %</td>
<td>--</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>Value</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>439.9</td>
<td>430.2</td>
<td>314.4</td>
</tr>
<tr>
<td></td>
<td>Difference</td>
<td>-2.2 %</td>
<td>--</td>
</tr>
</tbody>
</table>

With a shielded glow plug configuration as shown in figure 7.7, the methane jet even does not directly impinge onto the glow plug. Under this situation, the shock wave will have a negligible impact on ignition process near glow plug, which is the main focus for this research.

Therefore in the research of this thesis for gas flow in the combustion chamber and fuel ignition near glow plug, the shock wave phenomenon is not studied by using the relatively coarse mesh in order to reduce the computational load to an affordable level.
Appendix E

Nozzle Wall Friction Effect on Mass Flow Rate

A set of simulations was conducted to research the wall friction effect of the nozzle on the mass flow rate. To reduce the computational load, the simplified domain of a round duct was chosen to represent the nozzle injection flow.

The diameter of the round duct was fixed to be $D = 0.5$ mm. The duct length $L$ was selected for the simulation, which changes the overall friction of the duct wall to the flow passing through it. $L=1.6$ mm is the length of the nozzle for the injector in this research. Stagnation boundary conditions of $P_0 = 11$ MPa and $T_0 = 297$ K were applied on one end of the duct to represent the high-pressure reservoir. These values of pressure and temperature were kept constant for all of the simulations. At the discharge end of the duct, a low-pressure boundary condition was applied to represent the low-pressure reservoir. The pressure at the low pressure reservoir $P_{ex}$ was changed to different levels in each case of the simulations for each duct length. The temperature of the low pressure reservoir was kept to be a fixed value of $T_{ex} = 297$ K.
The result of the simulations is shown in figure E.1. In this figure, the x-axis is chosen to be the ratio of the simulation mass flow rate \( G \) to the theoretical mass flow rate \( G^* \), which is derived from 1-D isentropic flow without wall friction considered; the y-axis is chosen to be the pressure ratio of the low pressure reservoir to the fixed high pressure reservoir. Mass flow rate ratios are plotted for the five duct lengths simulated.

![Figure E.1](image)

Figure E.1  Simulation result of wall friction effect on the mass flow rate through a round duct of 0.5 mm diameter with 11MPa of \( P_0 \) and various \( P_{ex} \). \( G \) is the mass flow rate, \( G^* \) is the theoretical mass flow rate of 1-D isentropic flow.

For a given duct length, figure E.1 shows that when the low pressure reservoir is near to the high pressure reservoir, the mass flow rate is very small since the source of the flow motion, the pressure difference between the two ends, is small and the wall friction is substantial. As the pressure difference increases (the pressure ratio of \( P_{ex} \) to \( P_0 \) decreases), the mass flow rate increases fast. As the pressure difference increases to a certain value, it is high enough to
overcome wall friction to the flow, and the mass flow rate reaches its maximum value. After this, even though the pressure difference keeps on increasing, the flow is choked to this maximum mass flow rate.

To compare different length of the duct between different flow curves, figure E.1 shows that as the duct length increase, the maximum choking mass flow rate decreases, since the wall friction is larger.

This simulation result clearly shows the friction effect of the duct wall to the mass flow rate through the duct. It shows the same curve patterns and friction trends with the calculation result from Lapple charts by Levenspiel [1977].
Appendix F

Glow Plug Heat Transfer Analysis in Engine Environment

This appendix conducts the detailed calculation of the glow plug heat transfer analysis in engine environment discussed in chapter 5. It includes the calculations for convective heat transfer and Biot number listed in table 5-1, and analytical calculation for temperature drop by lumped heat capacitance method in section 5.3.

F.1. Calculations for Convective Heat Transfer and Biot Number

In the engine environment, the glow plug heating tube surface experiences convective cooling and heating that varies as the engine cycle progresses. Two cooling situations were evaluated for the glow plug convective heat transfer: cooling by intake air and cooling by injected methane jet as summarized in table 5-1.

For the case of glow plug cooling by injected methane jet, two cases were considered for two nozzle diameters: 0.34 mm and 0.50 mm.
F.1.1. Cooling by Intake Air

When the cold air is induced from inlet valves in the engine cylinder, the glow plug is experienced a convective cooling by the swirl motion of the cold air. The velocity of the cold air to glow plug is about 8 m/s from the swirl analysis in chapter 4. The temperature and the pressure of the cold air can be evaluated as 300 K and 101 kPa respectively.

To conduct the convective heat transfer analysis, the film temperature needs to be evaluated first:

\[ T_{\text{film}} = \frac{T_\infty + T_s}{2} = \frac{300K + 1200K}{2} = 750K \]  
Equation (F-1)

where: \( T_\infty \) is the gas temperature surrounding the glow plug;

\( T_s \) is the glow plug surface temperature.

So the Reynolds number can be evaluated as:

\[ \text{Re} = \frac{\rho \cdot V \cdot D}{\mu} = \frac{V \cdot D}{\nu} = \frac{(8\text{ m/s}) \times (0.005\text{ m})}{76.37 \times 10^{-6} \text{ m}^2 / \text{s}} = 523.8 \]  
Equation (F-2)

where: \( V \) is the gas velocity passing the glow plug;

\( D \) is the diameter of the glow plug;

\( \rho, \mu, \nu \) are the properties of the surrounding gas at film temperature, they are density, viscosity and kinematic viscosity respectively.

The Hilpert correlation was used for evaluating Nusselt number [Incropera and deWitt, 1996]:

\[ \overline{Nu}_D = \frac{\bar{h} \cdot D}{k} = C \cdot \text{Re}^m \cdot \text{Pr}^{1/3} \]  
Equation (F-3)

\[ \overline{Nu}_D = (0.683) \times (523.8)^{0.466} \times (0.702)^{1/3} = 11.23 \]

where: \( Pr \) is the Prandtl number of the surrounding gas at film temperature.
\( k \) is the thermal conductivity of the surrounding gas at film temperature.

\( C \) and \( m \) are the constants in Hilpert correlation determined by Reynolds number, they are 0.683 and 0.466 respectively for this case.

\( \bar{h} \) is the convective heat transfer coefficient for the glow plug.

From equation (F-2), \( \bar{h} \) can be derived as:

\[
\bar{h} = \frac{k}{D} \cdot \frac{\overline{N_u D}}{0.005m} = \frac{54.9 \times 10^{-3} W/(mK)}{0.005m} \times 11.23 = 123.3 \ (W/m^2-K)
\]

So Biot number can be derived as:

\[
Bi = \frac{\bar{h} \cdot L_c}{k_c} = \frac{(123.3 W/m^2 K) \cdot (0.75 \times 10^{-3} m)}{27.6 W/mK} = 0.0034 \quad \text{Equation (F-4)}
\]

where: \( L_c \) is outer shell thickness of the glow plug protective tube.

\( k_c \) is the thermal conductivity of glow plug protective tube – Inconel 750 at 1200 K

F.1.2. Cooling by Injected Methane Jet through a Small Nozzle

When the injected methane jet from a small nozzle of 0.34 mm diameter impinges onto the glow plug near to TDC, the glow plug experiences a strong convective heat loss. The properties of the fuel air mixture over the glow plug location at about 2ms are as follows:

\( P = 4000 \) kPa,
\( T = 683 \) K
\( V = 51.5 \) m/s
\( \rho = 17.9 \) kg/m³
\( X_{CH4} = 0.2639 \)

where: \( X_{CH4} \) is the mole fraction of methane in the mixture.

Thus, similar to equation (F-1), the film temperature is:
\[
T_{\text{film}} = \frac{T_m + T_s}{2} = \frac{683K + 1200K}{2} = 942K
\]

Based on the mole fraction of methane in the mixture the film temperature, following properties can be found:

\[Pr = 0.71\]

\[k = 0.064 \text{ (W/m-K)}\]

\[\mu = 35.7 \times 10^{-6} \text{ (N} \cdot \text{s/m}^2)\]

Notes: 1. There is lack of data for thermal conductivity \(k\) for methane at high temperature, but at low temperature of 100-500 K, it is comparable to the \(k\) for air with 16.6\% of the difference. Considering the small percentage of methane in the mixture, the thermal conductivity \(k\) for air at film temperature is used to estimate the \(k\) for the mixture.

2. Viscosity of the mixture is based on the equation from Touloukian et al [1979].

\[\mu^{-0.5} = X_{CH4} \cdot \mu_{CH4}^{-0.5} + X_{air} \cdot \mu_{air}^{-0.5}\]

So similar to equation (F-2), (F-3), and (F-4)

\[
Re = \frac{\rho \cdot V \cdot D}{\mu} = \frac{(17.9\text{ kg/m}^3) \times (8\text{ m/s}) \times (0.005m)}{35.7 \times 10^{-6} \text{ m}^2 / \text{s}} = 129327
\]

\[\bar{Nu}_D = \frac{h \cdot D}{k} = C \cdot \text{Re}^m \cdot Pr^{1/3} = 0.027 \times 129327^{0.805} \times 0.71^{1/3} = 313.9\]

where: \(C = 0.027, m = 0.905\)

\[\bar{h} = \frac{k}{D} \cdot \bar{Nu}_D = \frac{0.064W/(mK)}{0.005m} \times 313.9 = 4017.9 \quad (W/m^2K)\]

\[Bi = \frac{\bar{h} \cdot L}{k_c} = \frac{(4017.9W/m^2K) \times (0.75 \times 10^{-3}m)}{27.6W/mK} = 0.109\]
F.1.3. Cooling by Injected Methane Jet through a Large Nozzle

Similar to a small nozzle of 0.34 mm diameter, for a large nozzle of 0.50 mm diameter, the properties of the fuel air mixture over the glow plug location at about 5 ms are as follows:

\[ P = 4000 \text{ kPa}, \]
\[ T = 627 \text{ K}, \]
\[ V = 92.4 \text{ m/s}, \]
\[ \rho = 18.5 \text{ kg/m}^3, \]
\[ X_{CH_4} = 0.3713 \]

Thus, the film temperature is:

\[ T_{film} = \frac{T_{\infty} + T_s}{2} = \frac{627K + 1200K}{2} = 914K \]

Based on the mole fraction of methane in the mixture the film temperature, following properties can be found:

\[ Pr = 0.71 \]
\[ k = 0.062 \text{ (W/m-K)} \]
\[ \mu = 33.0 \times 10^{-6} \text{ (N\cdot s/m}^2\text{)} \]

Thus, also similar to equation (F-2), (F-3), and (F-4)

\[ Re = \frac{\rho \cdot V \cdot D}{\mu} = \frac{(18.5\text{kg/m}^3) \times (92.4\text{m/s}) \times (0.005\text{m})}{33.0 \times 10^{-6} \text{m}^2/\text{s}} = 258666 \]

\[ \frac{\overline{h} \cdot D}{k} = C \cdot Re^{m} \cdot Pr^{1/3} = 0.027 \times 258666^{0.805} \times 0.71^{1/3} = 548.3 \]

where: \( C = 0.027, m = 0.905 \)

\[ \overline{h} = \frac{k}{D} \cdot \frac{\overline{Nu}_D}{0.005m} \times 548.3 \times 6799.3 = 6799.3 \text{ (W/m}^2\text{-K)} \]
F.2. Analytical Calculation for Temperature Drop by Lumped Heat Capacitance Method under Natural Convection

F.2.1. The Governing Equation

When the power is turned off for the glow plug, it undergoes the natural convection in still air to cool down. From the theoretical analysis of a lumped heat capacitance model with only natural convection, the governing equation is [Incropera and deWitt, 1996]:

\[ T - T_\infty = (T_i - T_\infty) \cdot \exp(-Bi \cdot Fo) \]  

Equation (F-5)

where:  
- \( T_\infty \) is the surrounding air temperature;  
- \( T_i \) is the initial temperature of the glow plug;  
- \( Bi \) is the Biot number;  
- \( Fo \) is the Fourier number.

F.2.2. Evaluation of Bi for Lumped Heat Capacitance Method by Empirical Data

For the vertical cylinder with spherical cup end, Re, Nu, thus Bi and Fo can be empirically estimated [Rohsenow et al., 1998]

\[ Nu = \bar{h} \cdot D / k \]  

Equation (F-6)

\[ Ra = \frac{g \cdot \beta \cdot \Delta T \cdot D^3}{\nu \cdot \alpha} \]  

Equation (F-7)

where \( Ra \) is Rayleigh number.
From the empirical data, as $L/D = 20mm/5mm = 4$, $Nu_{cond}=1.05$, $G=0.695$, $n=1.07$, $C_j=0.103$ at $Pr=1.07$ for air, $m=10$.

Since $T_i=1200$ K, $T_\infty=300$ K, $\beta=1/ T_\infty$, from equation (F-7)

$$Ra = \frac{(9.807m / s^2) \times (1/300K) \times (1200K - 300K) \times (0.005m)^3}{(76.37 \times 10^{-6} m^2 / s) \times (109 \times 10^{-6} m^2 / s)} = 441.8$$

where: $\nu$ and $\alpha$ are kinematic viscosity and thermal diffusivity of air at film temperature $T_f = (T_i + T_\infty) = 750$ K.

$$Nu^T = G \times C_j \times Ra^{1/4} = 0.695 \times 0.103 \times 441.8^{1/4} = 0.328$$

where superscript $T$ stands for thick film.

$$Nu_l = \left[(Nu_{cond})^n + (Nu^T)^n\right]^{1/n} = \left[(1.05)^{1.07} + (0.328)^{1.07}\right]^{1/1.07} = 1.33$$

where subscript $l$ stands for laminar.

$$Nu_t = C_j \times Ra^{1/3} = 0.103 \times 441.8^{1/3} = 0.784$$

where subscript $t$ stands for turbulent.

$$Nu = \left[Nu_l^m + Nu_t^m\right]^{1/m} = [1.33^{10} + 0.784^{10}]^{1/10} = 1.331$$

From equation (F-6), $\overline{h}$ can be derived:

$$\overline{h} = \frac{k}{D} \times Nu = \frac{54.9 \times 10^{-3} W/(mK)}{0.005m} \times 1.331 = 14.61 \ W/(m^2K)$$
where \( k \) is the thermal conductivity of air at film temperature.

\[
Bi = \frac{\bar{h} \cdot r_0}{k_c} = \frac{(14.61 W/m^2 K) \times (0.0025 m)}{11.2 W/mK} = 0.003
\]

where \( k_c \) is the thermal conductivity of Inconel 601 (GP Shell) at room temperature. Noted that this is the approximate estimation, where taking the whole cylinder of the glow plug as a solid one with the same property as the outer shell of Inconel.

After evaluation of \( Bi \) in free air, \( Bi << 0.1 \), so it is acceptable to use lumped heat capacitance method.

**F.2.3. Recalculation of \( Bi \) by Evaluating Thermal Resistances**

![Diagram of system thermal resistances for glow plug](image)

Figure F.1  The illustration of system thermal resistances for glow plug

For our case, \( L=0.02 \text{ m} \), \( r_1=0.0015 \text{ m} \), \( r_2=0.0020 \text{ m} \), \( r_3=0.0025 \text{ m} \), the overall thermal resistance of the system is:

\[
R = R_{\text{cond}} + R_{\text{conv}} \quad \text{Equation (F-8)}
\]
\[ R_{\text{cond}} = R_{1-2} + R_{2} + R_{2-3} + R_{3} \quad \text{Equation (F-9)} \]

where \( R_2 \) and \( R_3 \) are the thermal resistance for MgO insulation and Inconel outer shell respectively. \( R_2 = \frac{\ln(r_2 / r_1)}{2\pi L k_2} \), \( R_3 = \frac{\ln(r_3 / r_2)}{2\pi L k_3} \).

\( k_2 \) is the thermal conductivity for MgO, \( k_2 = 11.1 \) W/(m-K)

\( k_3 \) is the thermal conductivity for Inconel 601, \( k_3 = 23.9 \) W/(m-K)

\( R_{1-2} \) and \( R_{2-3} \) are the thermal contact resistance for the surface between \( r_1 \) to \( r_2 \), and \( r_2 \) to \( r_3 \).

\[ R_{1-2} = R_{1-2} \pi r_1 L, \quad R_{2-3} = R_{2-3} \pi r_2 L. \quad \text{For our case, take } R_{1-2}^{'} = R_{2-3}^{'} = 0.2 \times 10^{-4} \text{ m}^2 \text{-K/W}. \]

\( R_{\text{conv}} \) is the thermal resistance for convection. \( R_{\text{conv}} = \frac{1}{2\pi r_3 L h} = 218.02 \text{ (K/W)} \)

So equation (F-9) can be substituted by

\[ R_{\text{cond}} = R_{1-2} + R_{2} + R_{2-3} + R_{3} = 0.212 + 0.206 + 0.159 + 0.074 = 0.651 \text{ (K/W)} \]

\[ Bi = \frac{R_{\text{cond}}}{R_{\text{conv}}} = \frac{0.651}{218.02} = 2.99 \times 10^{-3} \quad \text{Equation (F-10)} \]

**F.2.4. Estimation of the Temperature Drop**

\[ Fo = \frac{\alpha \cdot t}{r_1^2} = \frac{3.4 \times 10^{-6} \text{ m}^2 / \text{s}}{(0.0015 \text{ m})^2} \times 1.511t \]

where \( \alpha \) is the thermal diffusivity of Inconel at 300 K.

From equation (F-5), at \( t=30 \text{ second} \), the temperature will drop from initial 970 K to the new temperature \( T \):
\[ T = T_{\infty} + (T_i - T_{\infty}) \cdot \exp(-Bi \cdot Fo) = 300 + (970 - 300) \times \exp(-2.99 \times 10^{-3} \times 1.511 \times 30) \]

= 885 (K)

This shows that it has a large difference with the experimental result of which the temperature drop is to 410 K. This implies that there is another source of heat loss which is un-negligible, that is – the radiation heat loss, which has large effect on the heat loss especially at high temperature.
Appendix G

Modifications on Turbulent Mixing-Controlled Chemistry and Tuning of the Kinetic Reaction Constants

In KIVA3-V code, there are 4 kinetic and 6 equilibrium built-in reactions to model the chemical reactions for ignition and combustion, and there is a turbulent mixing-controlled chemistry to model the fast flame propagation under turbulent condition. However, these models were originally designed for conventional liquid fuel powered engines. So, for simulating methane ignition and combustion processes, some modifications and tuning on the models of chemical reactions and turbulent mixing-control chemistry need to be conducted.

G.1. Modifications on Turbulent Mixing-Controlled Chemistry

There is a built-in turbulent mixing-controlled chemistry in KIVA3-V counting the turbulent effects on the combustion rate (physical controlled speed) in diffusive combustion phase. But in the ignition delay phase and the premixed combustion phase, the chemical reaction speed is the dominant speed, especially at the time before the ignition (ignition delay period).
However, the difference between the chemical and physical controlled reaction speed was not counted in the original KVIA code, i.e., the switch of the turbulent mixing-controlled chemistry can be turned on or off only for the whole phases of the injection and combustion, but not for the diffusive combustion phase [Amsden, 1993].

Because of the low temperature within the ignition delay time, the turbulent mixing-controlled chemistry will greatly increase the reaction speed (in order of 3 or 4 for some strong turbulent area compared to chemical reaction speed only). So it will overestimate the reaction speed if it is applied within the ignition delay phase, thus the computational ignition delay is shortened.

Suggested modifications by Micklow and Gong [2001] distinguished the combustion into 3 phases: The first phase is ignition delay. Within this period, only the kinetic chemical reaction speed determines the overall reaction speed. Since in this period the temperature is low (around 1000K), the chemical reaction speed is also very low. The second phase is premixed combustion, starting from the ignition occurs. The criterion for ignition is local temperature great than 2000 K. As suggested by Micklow and Gong, the period of premixed combustion is input as experience and engine configurations, and to be claimed is nearly a constant under different engine working state. The third phase is diffusive combustion after the premixed combustion. Within this phase, the overall speed is the maximum of kinetic reaction speed (chemical controlled speed) and turbulent mixing-controlled speed (physical controlled speed).

For the research work in this thesis, some modifications on turbulent mixing-controlled chemistry were conducted as suggested by Micklow and Gong [2001]. Besides these, some improvement was also made for the premixed period: after the ignition, in the region where the local temperature is less than 2000K or the turbulent is not strong, only the kinetic reaction speed
applies, since it is treated as premixed combustion. Meanwhile, in the region where the local temperature is more than 2000K and the turbulent is strong, it is considered as diffusion combustion, the reaction speed is chosen to be the maximum of kinetic reaction speed (chemical controlled speed) and turbulent mixing-controlled speed (physical controlled speed).

G.2. Tuning of the Kinetic Reaction Equations

The KIVA code builds in four 4 kinetic reactions and 6 equilibrium reactions which involve 12 species (CH$_4$, O$_2$, N$_2$, CO$_2$, H$_2$O, H, H$_2$, O, N, OH, CO, NO). The fuel oxidation reaction for methane is chosen as one-step reaction:

$$\text{CH}_4 + \text{O}_2 \Rightarrow \text{CO}_2 + \text{H}_2\text{O} + q$$

$q$ is the volumetric energy released from this chemical reaction.

$$\dot{q} = Q \cdot \omega$$

where: $Q$ is low heating value (LHV) of methane, in unit of [J/mole]

$
\omega_r$ is speed of the kinetic reaction for methane oxidization.

$$\dot{\omega} = k_f \cdot \left( \frac{\rho_{CH_4}}{W_{CH_4}} \right)^{a_{CH_4}} \cdot \left( \frac{\rho_{O_2}}{W_{O_2}} \right)^{a_{O_2}}$$

where $W_{O_2}$, $W_{CH_4}$, $\rho_{O_2}$, and $\rho_{CH_4}$ are the molecular weight and density for O$_2$ and CH$_4$ respectively.

$k_f$ is the forward rate coefficients for the reaction and is assumed to be of a generalized Arrhenius form (noted that the backward rate for the reaction of methane oxidization is zero):

$$k_f = A_f \cdot T^{\frac{E_f}{T}} \cdot \exp\left(\frac{-E_f}{T}\right)$$
where: $E_f$ is activation temperature (in Kelvin); $A_f$ and $\zeta_f$ are the forward coefficients.

So, in the volumetric energy release $q$, there are five constants need to be assigned to the proper values according to experimental or empirical data: is activation temperature (in Kelvin); $A_f$, $\zeta_f$, $E_f$, $a'_{CH4}$, and $a'_{O2}$.

There are two sets of available data used upon comparison in this thesis for the tuning process of the constants in the chemical reaction for methane oxidation. The first is a dynamic modeling results by Naber et al. [1994], they conducted a series of experiments to test the ignition delays under the conditions of natural gas injection into combustion chamber with constant density of air (20.4 kg/m$^3$) at different initial temperatures. They analyzed the physical delay time for their experimental apparatus, and subtracted this physical delay from the experimental ignition delays and concluded the chemical ignition delays. The second is static modeling results by Agarwal and Assanis [1997], they used chemical modeling package of Skeletal, DRM 22, and GRI Mech 1.2 to compute the ignition delays under the conditions of the quiescent stoichemetric methane and air mixture for constant density of 20.4 kg/m$^3$ at different initial temperatures. These results are shown in figure G.1.

When using the set of chemical constants in Sun’s work [1999], which is also suggested by KIVA for methane, to computer the ignition delays, they are 10 to 100 times higher than the experimental data provided in [Naber et al., 1994], and the analytical and computational data in [Agarwal and Assanis, 1997]. This is also shown in figure G.1.

The reason for the large discrepancy is believed to be that the calibration for original KIVA-3V kinetic reaction coefficients is based on the normal engine situation developed for liquid furls, especially with the turbulent mixing-controlled chemistry always turned on, which
will significantly over-estimate the chemical reaction speed. But when at computation in initial quiescent state clearly shows the disabled effect of turbulent mixing-controlled chemistry on ignition delay by no turbulence even it is turned on. As a conclusion, the chemical reaction coefficients have to be re-calibrated for the KIVA-3V kinetic reaction equations for methane injection and ignition.

The new set of the chemical reaction coefficient was tuned under Naber’s experimental conditions and compared to. The tuning result is shown in figure G.1, the result illustrates that the tuned new set of constants can reflects the chemical reaction speed compared to the Naber’s chemical ignition delay from the experiments, and to the Agarwal’s numerical modeling. However, it has to be compromised to the low or high temperature ends. This fit can be improved if a two-step chemical reaction model for methane oxidation is implemented in the future research.

**Ignition Delay of Methane vs. Temperature**

![Ignition Delay of Methane vs. Temperature](image)

**Figure G.1** The tuning of the chemical reaction coefficients for methane as a fuel.
Appendix H

Effects of Elliptical Nozzle Shapes on Natural Gas Jet

The most interesting phenomenon of a jet from an elliptical nozzle is the axis switching. Spreading in the minor axis plane (the plane containing the minor axis of the nozzle) was much greater than that in the major-axis plane. Much research has been conducted on the elliptical nozzles [Ho and Gutmark, 1987; Hussain, 1989; Hussain, 1991]. Another expectation of an elliptical nozzle is that more air might be entrained into the jet compared to the round nozzle.

Experiments are currently being designed and carried at ERDL at University of Toronto although so far no final experimental data are available for comparison. Simple simulation of an elliptical nozzle was tried for the future analysis of the experiments. Some efforts were made to generate the elliptical nozzle using the KIVA mesh generator with modifications. The elliptical nozzle dimensions were set to be same as those in the experiments at ERDL. The major axis is 0.288 mm, and the minor axis is 0.144 mm with an aspect ratio of 2:1.

Figure H.1 shows the cross section outline of the fuel-air equivalence ratio of 1 for the jet at different distances from the nozzle exit after 0.93 ms of the injection. The axis-switching growth of the jet injected from an elliptical nozzle is clearly illustrated.
Simulations were conducted to compare the elliptical nozzle with an equivalent round nozzle (having the same nozzle area). The results show that they have nearly the same mass flow rate and jet penetration length.

Figure H.2 shows the fuel-air equivalence ratio ($\phi = 0\sim2.0$) and the temperature contours at the cross-section plane of the jet after 0.93 ms of injection for both the elliptical nozzle and the equivalent round nozzle. The plane is at the distance from the nozzle exit ($x$) of 1.0 cm. From the figure it can be seen that the results are almost identical for the elliptical nozzle and the equivalent round one. If more air had been entrained for the elliptical nozzle, the mixing area and temperature would have been much larger and higher. The identical results suggest that more air is not entrained into the jet. This could be further studied when experimental data are available.
Figure H.2  Comparison of the elliptical nozzle and the equivalent round one.
Appendix I

Preliminary Research On Pintle Valve Model

The poppet valve model of the injector produces a local high temperature zone below the valve moving face when the poppet valve opens. This is because the valve moves down relatively fast and compresses the air just below it. The highest computational local temperature can increase to over 1200K at the center of the valve bottom face, thus artificial ignition of the fuel air mixture may occur when computing using the KIVA code with turbulent mixing-controlled chemistry enabled, as shown in figure I.1.

To avoid this false ignition from the computational result, the turbulent mixing-controlled chemistry needed to be disabled before the local temperature reaches 2000 K as the threshold value of ignition determination. The detailed introduction and modification of the turbulent mixing-controlled chemistry is in Appendix G.1.
To further compare the differences of the flow characteristics between the poppet valve with a real injector pintle, a tapered pintle valve model was developed to simulate the real shape of the injector. It is more like the real pintle motion situation: when the pintle opens, unlike the valve moving downward, it is moving upward. The pintle valve model avoided the high temperature region generated from compression to the air in the injector by the poppet valve as shown in figure I.1.

Figure I.2 shows the shape of the pintle valve model which is similar to the real injector pintle. It has the same restriction area (smallest area at the seating place) with the poppet valve model.
Although the gas flow may be more restricted by the outline profile of the poppet valve than the pintle valve, when reaching the steady state, the pintle valve model still has similar trends for the temperature and fuel air equivalence ratio graphs as the poppet valve model shown in figure 4.3, and has similar velocity and Mach number profiles when the flow reaches the steady state as for the poppet valve model shown in figure 4.4. So the poppet valve model is qualified for qualitatively investigating the injector flow behavior, but not ignition.

A detailed comparison between the pintle valve and poppet valve at the early stage of the flow development is shown in figure I.3. Because of the flow restriction due to the valve profile, the pintle valve has less friction upstream within the injector and thus has less pressure and temperature fluctuation within the injector, especially for the temperature.

Figure I.3 Comparison of flow development at early injection stage for pressure and temperature between pintle valve model and poppet valve model.